Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 11:53 AM EDT

PDB ID	:	7M4W / pdb_00007m4w
EMDB ID	:	EMD-23668
Title	:	A. baumannii Ribosome-Eravacycline complex: Empty 70S
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2021-03-22
Resolution	:	2.55 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

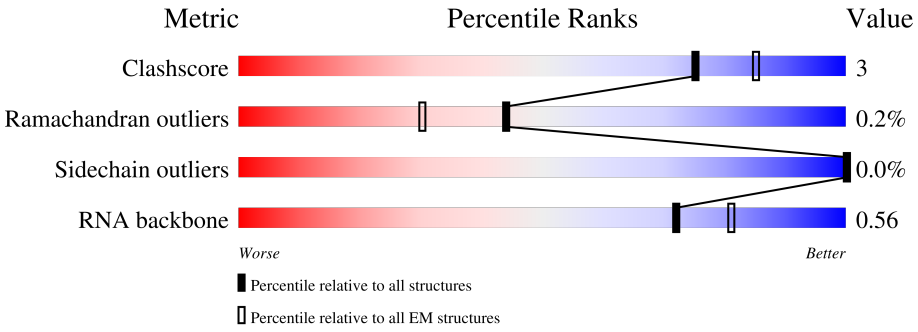
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

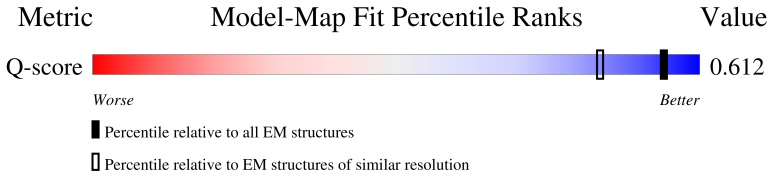
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.55 Å.

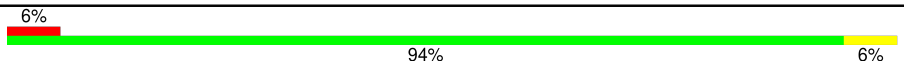
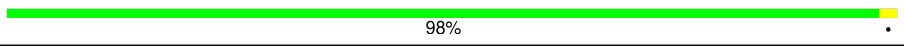
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





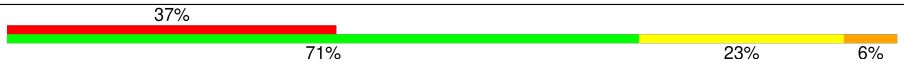
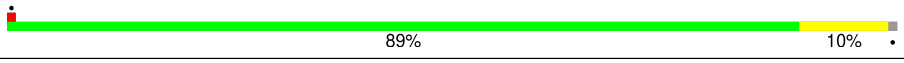
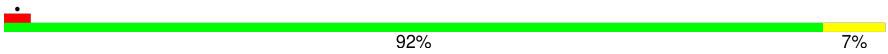
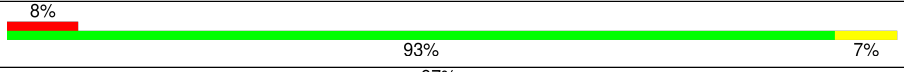
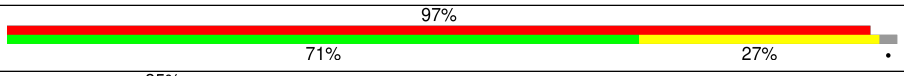
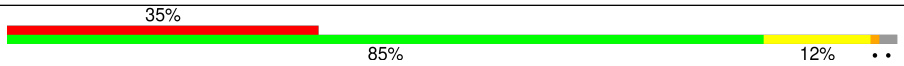
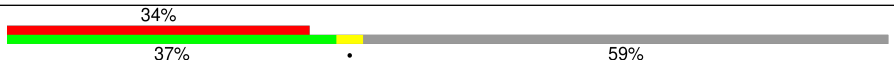
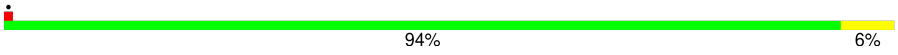
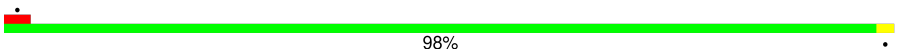
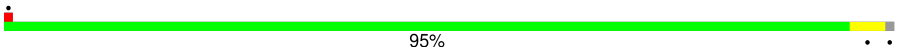
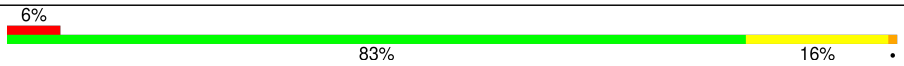
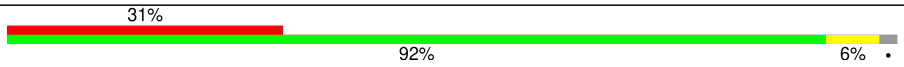
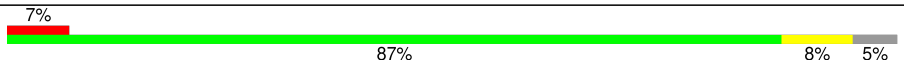
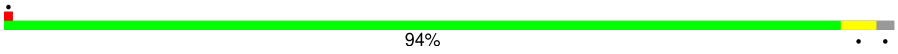
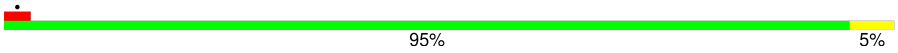
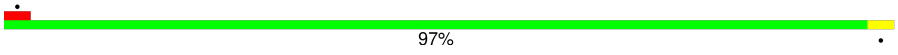
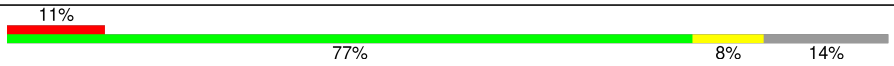
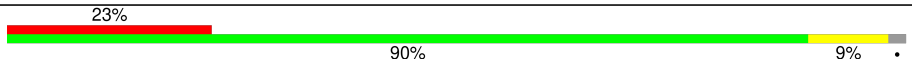
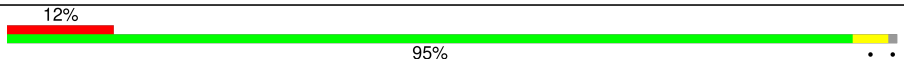
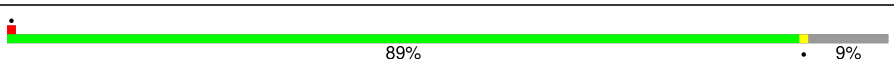
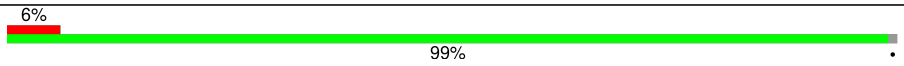
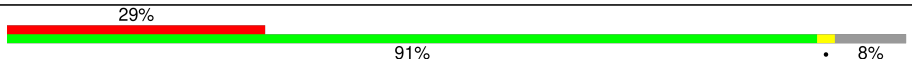
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7475 (2.05 - 3.05)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	51	
2	1	44	
3	2	64	

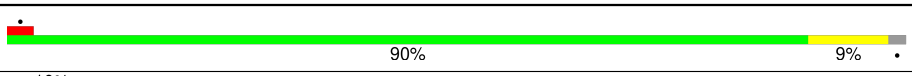
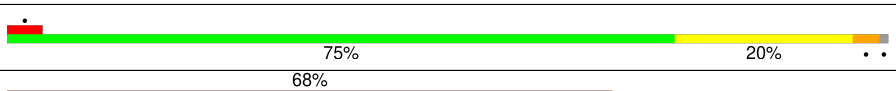
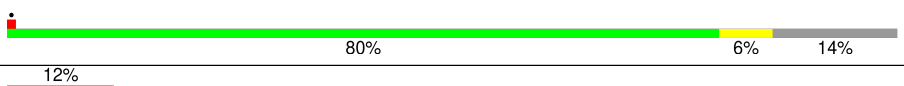
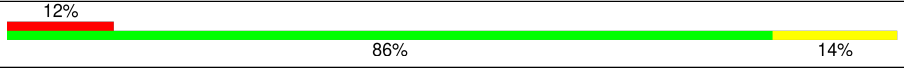
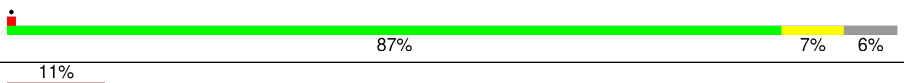
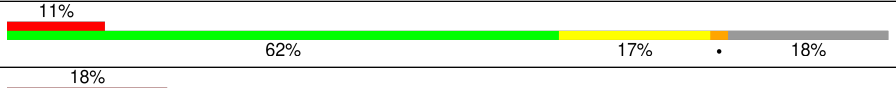
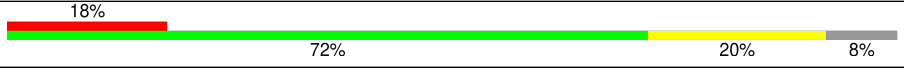
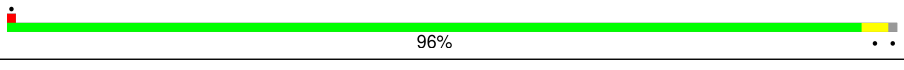
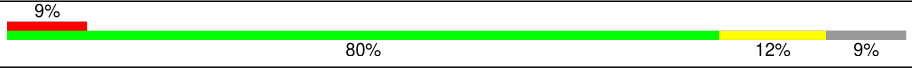
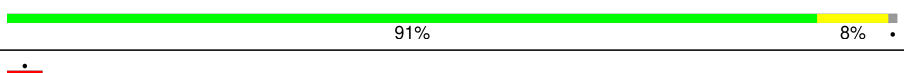
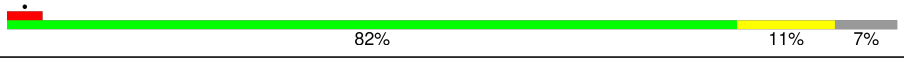
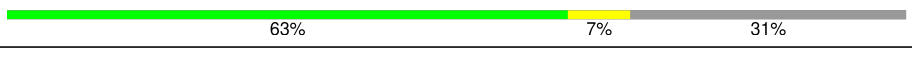
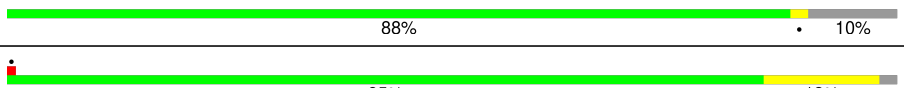
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Mol	Chain	Length	Quality of chain
4	3	38	
5	A	2918	
6	B	115	
7	C	274	
8	D	212	
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	

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Mol	Chain	Length	Quality of chain
29	Y	58	
30	Z	61	
31	a	1544	
32	b	250	
33	c	250	
34	d	208	
35	e	165	
36	f	127	
37	g	156	
38	h	131	
39	i	128	
40	j	103	
41	k	128	
42	l	124	
43	m	118	
44	n	101	
45	o	89	
46	p	101	
47	q	85	
48	r	75	
49	s	91	
50	t	88	
51	u	71	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 137923 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2730	Total	C	N	O	P	0	0
			58566	26143	10721	18972	2730		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	200	Total	C	N	O	S	0	0
			1516	952	281	278	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	174	Total	C	N	O	S	0	0
			1370	871	243	248	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total 946	C 592	N 180	O 169	S 5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	144	Total 1071	C 663	N 213	O 195	0	0

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total 1087	C 687	N 210	O 185	S 5	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total 942	C 590	N 186	O 163	S 3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total 857	C 528	N 173	O 155	S 1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	116	Total 913	C 575	N 176	O 162	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total 934	C 589	N 197	O 146	S 2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total	C	N	O	S	0	0
			710	452	128	129	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	T	103	Total	C	N	O	0	0
			766	476	142	148		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	77	Total	C	N	O	S	0	0
			585	363	112	108	2		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total	C	N	O	S	0	0
			632	395	130	105	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	60	Total	C	N	O	S	0	0
			486	302	93	90	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	57	Total	C	N	O	S	0	0
			455	281	87	84	3		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	55	Total	C	N	O	S	0	0
			456	271	102	82	1		

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1528	Total	C	N	O	P	0	0
			32782	14631	5994	10630	1527		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	225	Total	C	N	O	S	0	0
			1769	1110	328	325	6		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	104	Total	C	N	O	S	0	0
			867	546	158	159	4		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	143	Total	C	N	O	S	0	0
			1127	706	211	203	7		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	126	Total	C	N	O	S	0	0
			991	618	197	175	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	82	Total	C	N	O	S	0	0
			644	403	128	112	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	52	Total 426	C 273	N 74	O 79	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total 646	C 412	N 125	O 107	S 2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	86	Total 663	C 409	N 139	O 113	S 2	0	0

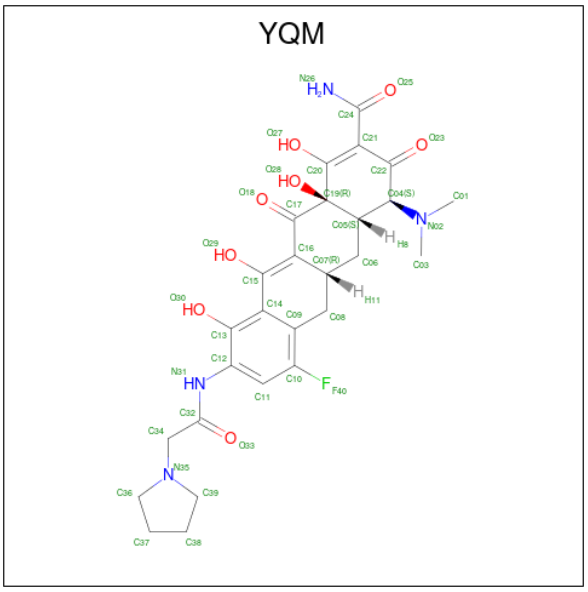
- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	63	Total 522	C 327	N 105	O 89	S 1	0	0

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	3	1	Total 1	Zn 1	0

- Molecule 53 is Eravacycline (CCD ID: YQM) (formula: $C_{27}H_{31}FN_4O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
53	A	1	Total C F N O 40 27 1 4 8	0
53	A	1	Total C F N O 40 27 1 4 8	0
53	a	1	Total C F N O 40 27 1 4 8	0

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
54	A	136	Total Mg 136 136	0
54	B	1	Total Mg 1 1	0
54	D	1	Total Mg 1 1	0
54	K	1	Total Mg 1 1	0
54	a	52	Total Mg 52 52	0

- Molecule 55 is water.

Mol	Chain	Residues	Atoms	AltConf
55	2	2	Total O 2 2	0

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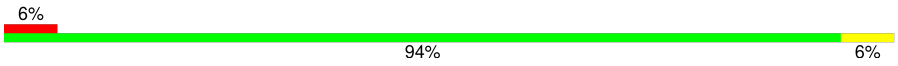
Mol	Chain	Residues	Atoms	AltConf
55	A	597	Total O 597 597	0
55	B	4	Total O 4 4	0
55	C	7	Total O 7 7	0
55	D	4	Total O 4 4	0
55	E	3	Total O 3 3	0
55	K	7	Total O 7 7	0
55	R	1	Total O 1 1	0
55	U	1	Total O 1 1	0
55	Z	2	Total O 2 2	0
55	a	156	Total O 156 156	0
55	i	2	Total O 2 2	0
55	j	3	Total O 3 3	0
55	k	1	Total O 1 1	0
55	m	1	Total O 1 1	0
55	n	3	Total O 3 3	0
55	q	1	Total O 1 1	0
55	s	1	Total O 1 1	0
55	t	1	Total O 1 1	0

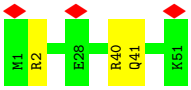
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S ribosomal protein L33

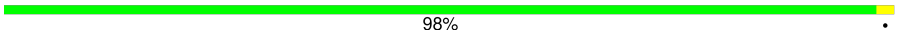
Chain 0:





- Molecule 2: 50S ribosomal protein L34

Chain 1:

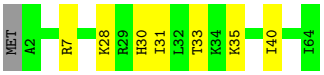




- Molecule 3: 50S ribosomal protein L35

Chain 2:





- Molecule 4: 50S ribosomal protein L36

Chain 3:

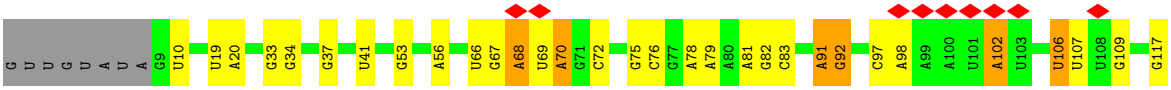


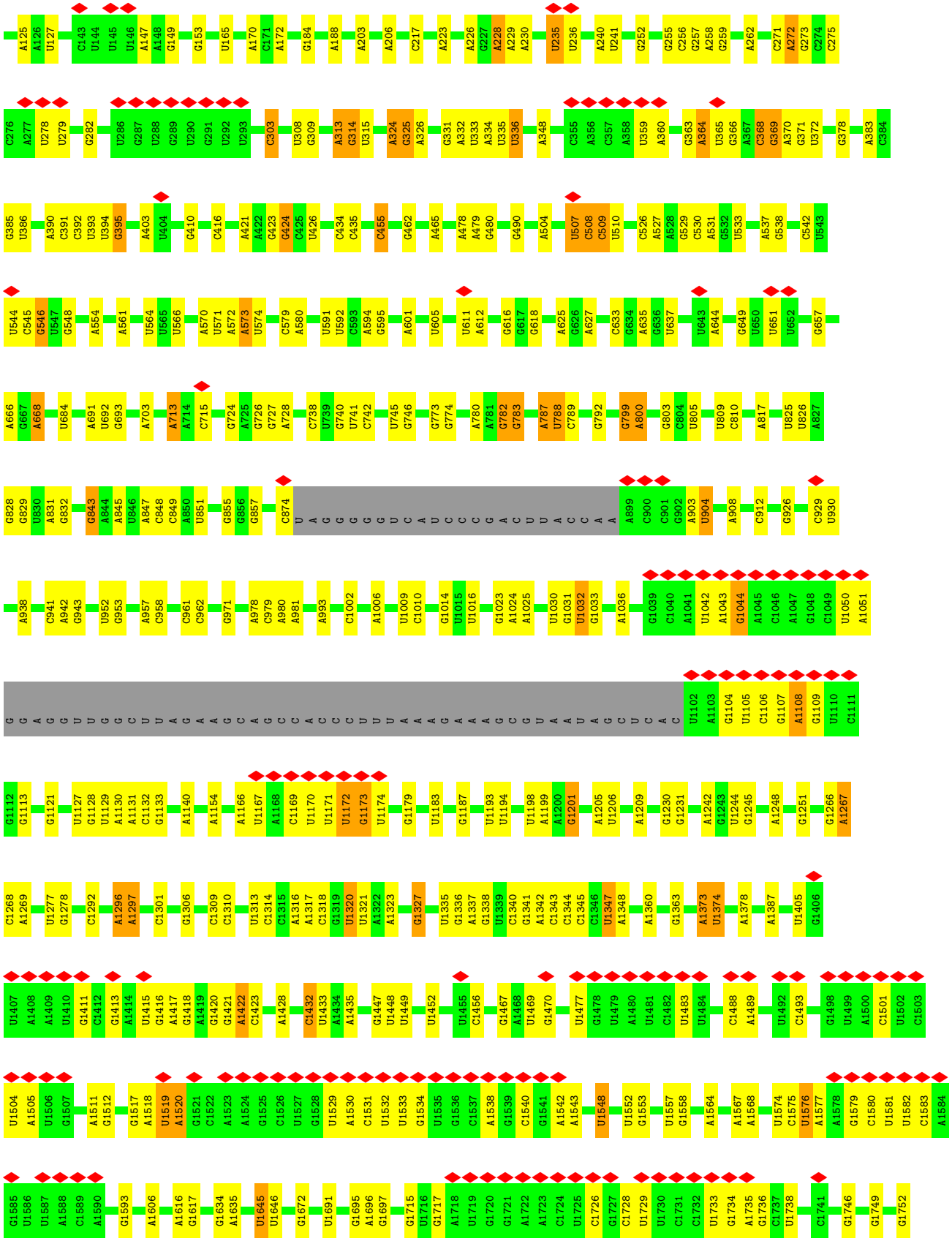


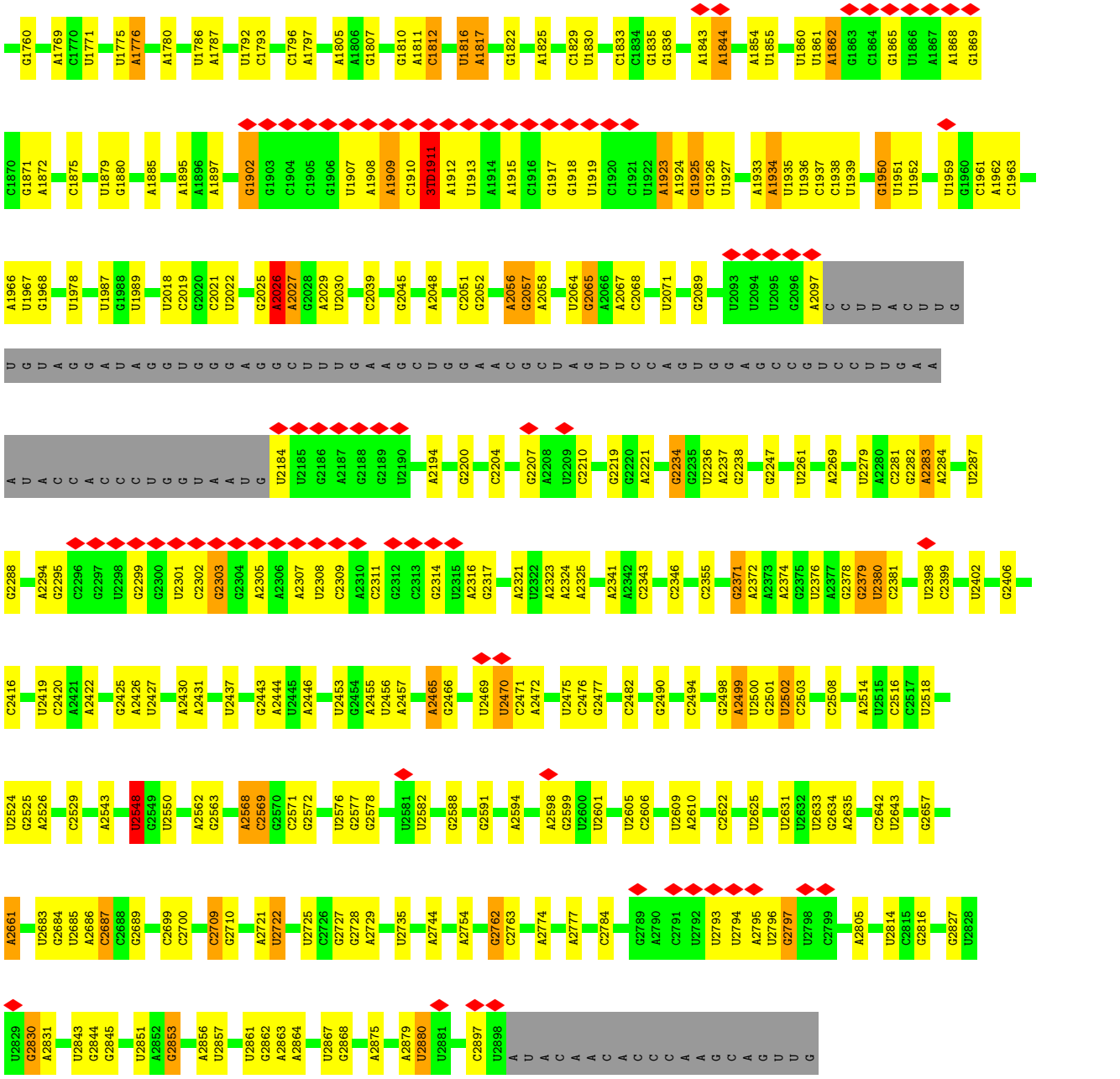
- Molecule 5: 23s ribosomal RNA

Chain A:





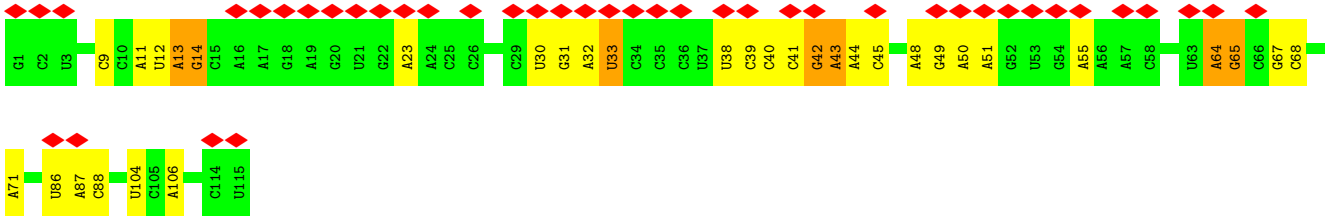

A125 A126 U127 C143 U144 U145 U146 A147 A148 G149 G153 U165 A170 C171 A172 G184 A188 A203 A206 C217 A223 A226 G227 A228 A229 A230 U235 U236 A240 U241 G252 C255 C256 G257 A258 G259 A262 C271 A272 G273 C274 C275
C276 A277 U278 U279 G282 U286 C287 U288 G289 U290 G291 U292 U293 C303 U308 G309 A313 G314 U315 A324 G325 A326 G331 A332 U333 A334 U335 U336 A348 C355 A356 C357 A358 U359 A360 G363 A364 U365 G366 A367 C368 G369 A370 G371 U372 G378 A383 C384
G385 U386 A390 C391 C392 U393 U394 G395 A403 U404 G410 C416 A421 A422 G423 G424 C425 U426 C434 C435 C455 G462 A465 A478 A479 G480 G490 A504 U507 C508 C509 U510 C526 A527 A528 G529 C530 A531 G532 U533 A537 G538 C542 U543
U544 C545 G546 U547 G548 A554 A561 U564 U565 U566 A570 U571 A572 A573 U574 C579 A580 U591 U592 C593 A594 G595 A601 U605 U611 A612 G616 G617 G618 A625 G626 A627 C633 G634 A635 G636 U637 U643 A644 G649 U650 U651 U652 G657
A666 G667 A668 U684 A691 U692 G693 A703 A713 A714 C715 G724 A725 G726 G727 A728 C738 U739 G740 U741 C742 U745 G746 G773 G774 A780 A781 G782 G783 A787 U788 C789 G792 G799 A800 G803 C804 U805 U809 C810 A817 U825 U826 A827
G828 G829 U830 A831 G832 G843 A844 A845 U846 A847 C848 C849 A850 U851 G855 G856 G857 C874 U A G G G G U C A U C C C G A C U U A C C A C A A899 C900 C901 G902 A903 U904 A908 C912 G926 C929 U930
A938 C941 A942 G943 U952 G953 A957 C958 C961 C962 G971 A978 C979 A980 A981 A993 C1002 A1006 U1009 C1010 G1014 U1015 U1016 G1023 A1024 A1025 U1030 G1031 U1032 G1033 A1036 G1039 C1040 A1041 U1042 A1043 G1044 A1045 C1046 A1047 G1048 C1049 U1050 A1051
G G A G G U U G G C U U G A G G A A G C A G G C C A G C C A C C C U U U A A A G A A A A G C C G U A A U A G C U C A C U1102 A1103 G1104 U1105 C1106 G1107 A1108 G1109 U1110 C1111
G1112 G1113 G1121 U1127 G1128 U1129 A1130 A1131 C1132 G1133 A1140 A1154 A1166 U1167 A1168 C1169 U1170 U1171 U1172 G1173 U1174 G1179 U1183 G1187 U1193 U1194 U1198 A1199 A1200 G1201 A1205 U1206 A1209 G1230 G1231 A1242 G1243 U1244 G1245 A1248 G1251 G1266 A1267
C1268 A1269 U1277 G1278 C1292 A1296 A1297 C1301 G1306 C1309 C1310 U1313 C1314 C1315 A1316 A1317 C1318 G1319 U1320 U1321 A1322 A1323 G1327 U1335 G1336 A1337 G1338 U1339 C1340 G1341 A1342 C1343 C1344 C1345 C1346 U1347 A1348 A1360 G1363 A1373 U1374 A1378 A1387 U1405 G1406
U1407 A1408 A1409 U1410 G1411 C1412 G1413 A1414 U1415 G1416 A1417 G1418 A1419 G1420 G1421 A1422 C1423 A1428 C1432 U1433 A1434 A1435 G1447 U1448 U1449 U1452 U1455 C1456 G1467 A1468 U1469 G1470 U1477 G1478 U1479 A1480 U1481 C1482 U1483 U1484 C1488 A1489 U1492 C1493 G1498 U1499 A1500 C1501 U1502 C1503
U1504 A1505 U1506 G1507 A1511 G1512 G1517 A1518 U1519 A1520 G1521 C1522 A1523 A1524 G1525 C1526 U1527 G1528 U1529 A1530 C1531 U1532 U1533 G1534 U1535 G1536 C1537 A1538 G1539 C1540 G1541 A1542 A1543 U1548 U1552 G1553 U1557 G1558 A1564 A1567 A1568 U1574 C1575 U1576 A1577 A1578 G1579 C1580 U1581 U1582 C1583 A1584
G1585 U1586 U1587 A1588 C1589 A1590 G1593 A1606 A1616 G1617 G1634 A1635 U1645 U1646 G1672 U1691 G1695 A1696 G1697 G1715 U1716 U1717 A1718 U1719 G1720 G1721 A1722 A1723 C1724 U1725 C1726 G1727 C1728 U1729 U1730 C1731 C1732 U1733 G1734 A1735 U1736 C1737 U1738 C1741 G1746 G1749 G1752



• Molecule 6: 5s ribosomal RNA

Chain B:

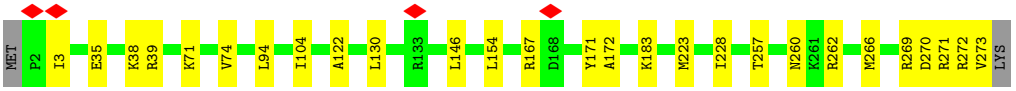




• Molecule 7: 50S ribosomal protein L2

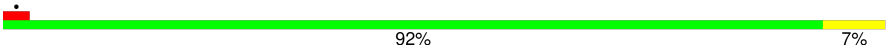
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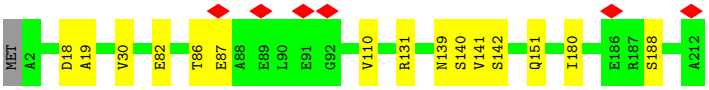




• Molecule 8: 50S ribosomal protein L3

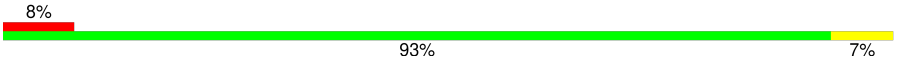
Chain D:

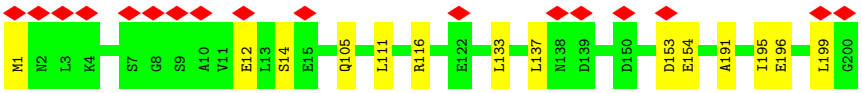




• Molecule 9: 50S ribosomal protein L4

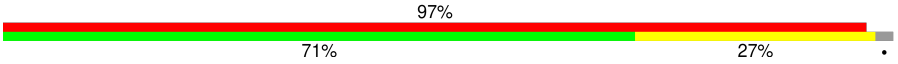
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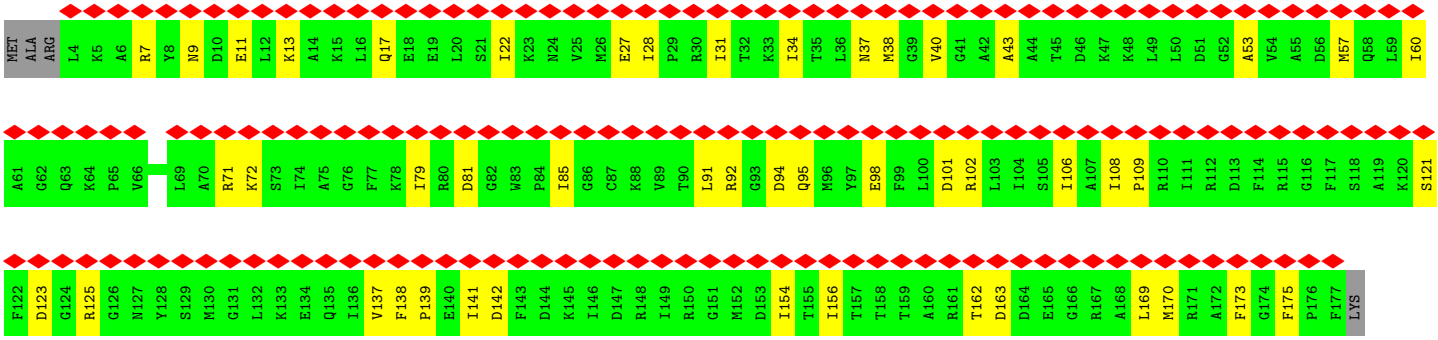




• Molecule 10: 50S ribosomal protein L5

Chain F:

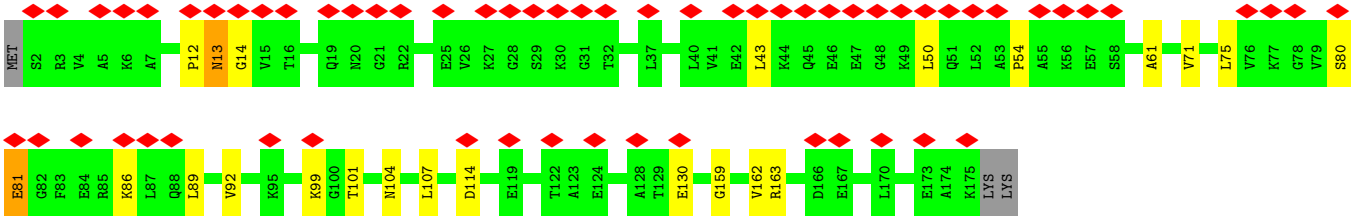




• Molecule 11: 50S ribosomal protein L6

Chain G:

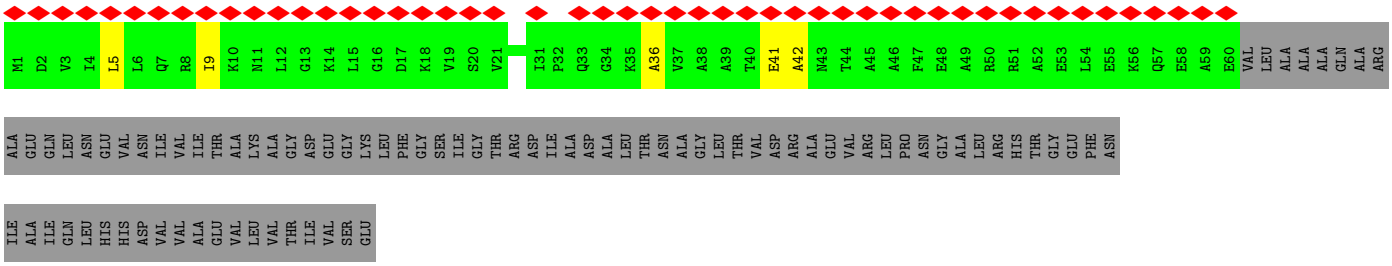




• Molecule 12: 50S ribosomal protein L9

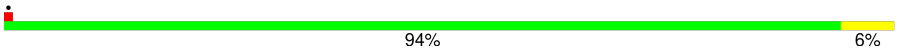
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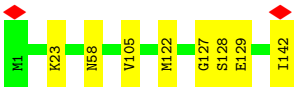




• Molecule 13: 50S ribosomal protein L13

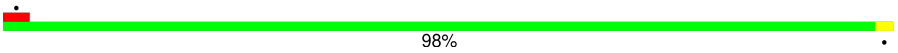
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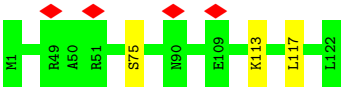




• Molecule 14: 50S ribosomal protein L14

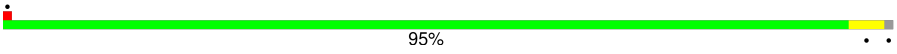
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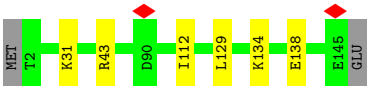




• Molecule 15: 50S ribosomal protein L15

Chain K:

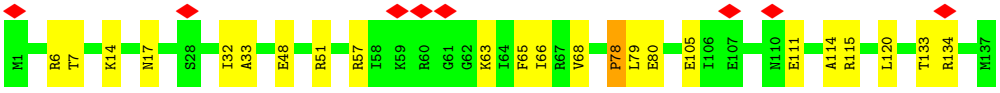




• Molecule 16: 50S ribosomal protein L16

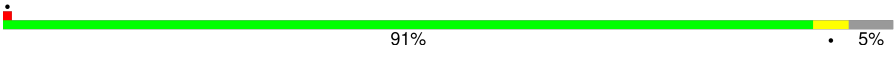
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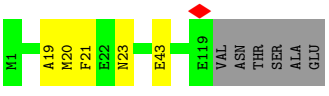




• Molecule 17: 50S ribosomal protein L17

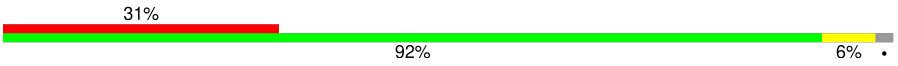
Chain M:

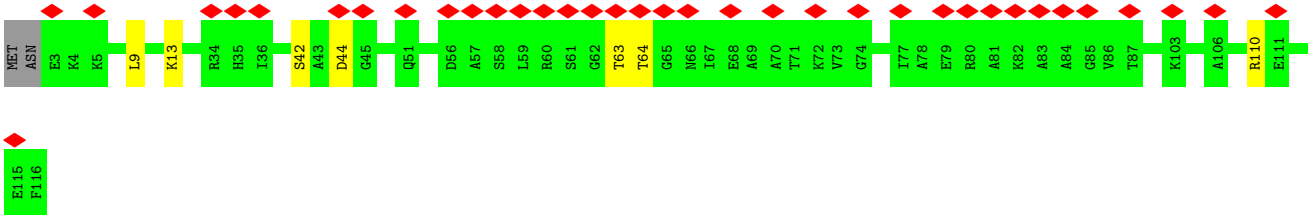




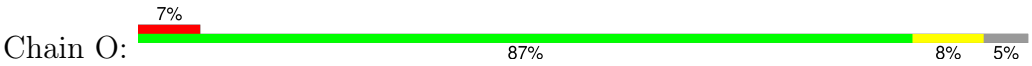
• Molecule 18: 50S ribosomal protein L18

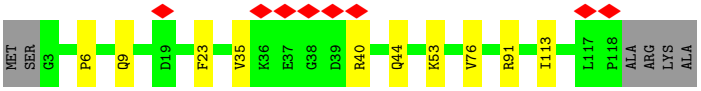
Chain N:





• Molecule 19: 50S ribosomal protein L19





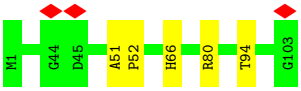
• Molecule 20: 50S ribosomal protein L20





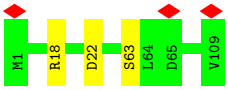
• Molecule 21: 50S ribosomal protein L21



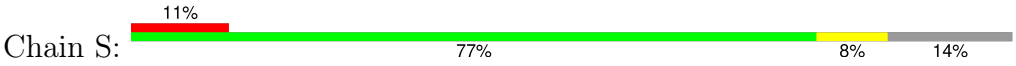


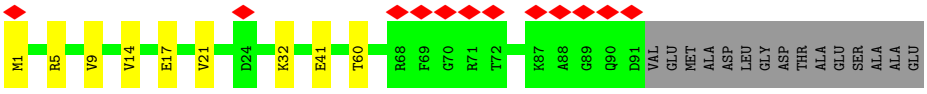
• Molecule 22: 50S ribosomal protein L22



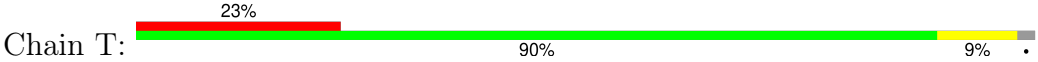


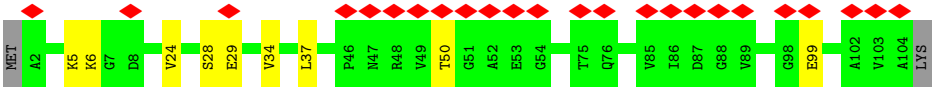
• Molecule 23: 50S ribosomal protein L23





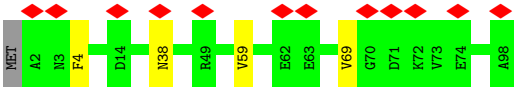
• Molecule 24: 50S ribosomal protein L24



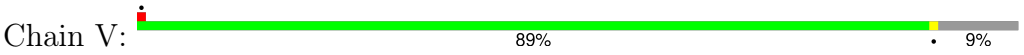


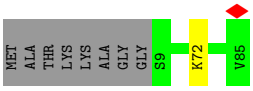
• Molecule 25: 50S ribosomal protein L25





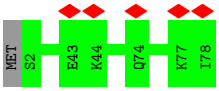
• Molecule 26: 50S ribosomal protein L27



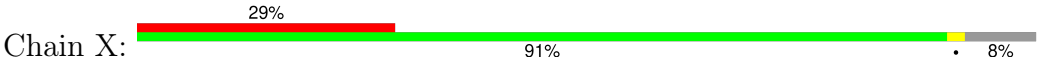


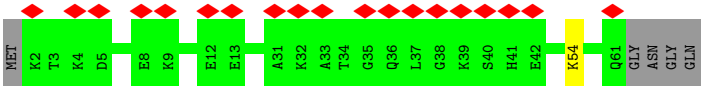
• Molecule 27: 50S ribosomal protein L28



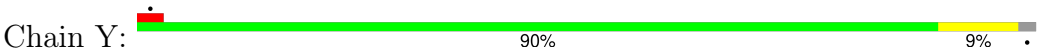


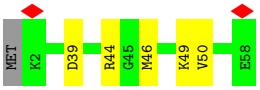
• Molecule 28: 50S ribosomal protein L29



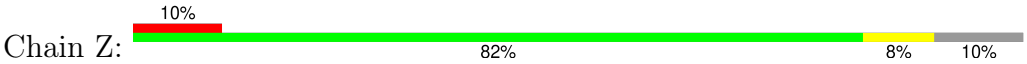


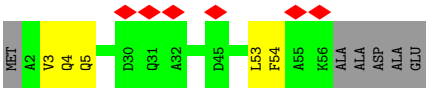
• Molecule 29: 50S ribosomal protein L30





• Molecule 30: 50S ribosomal protein L32

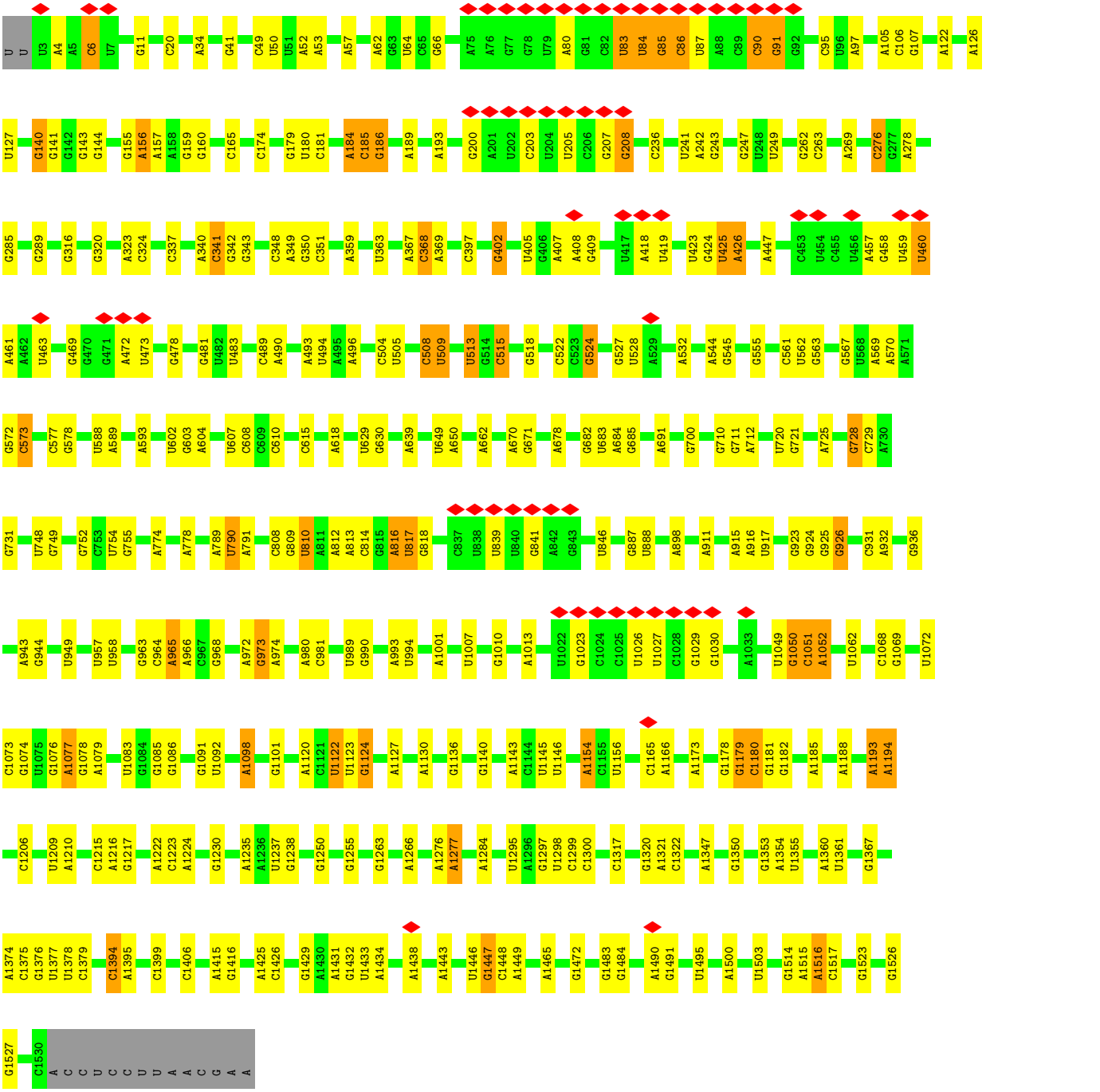




• Molecule 31: 16s Ribosomal RNA

Chain a:

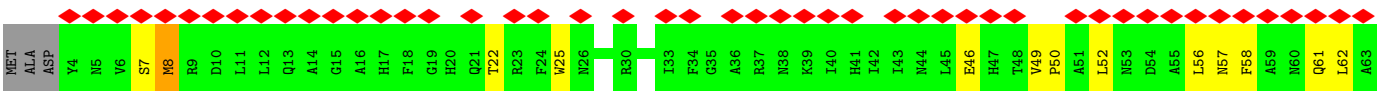


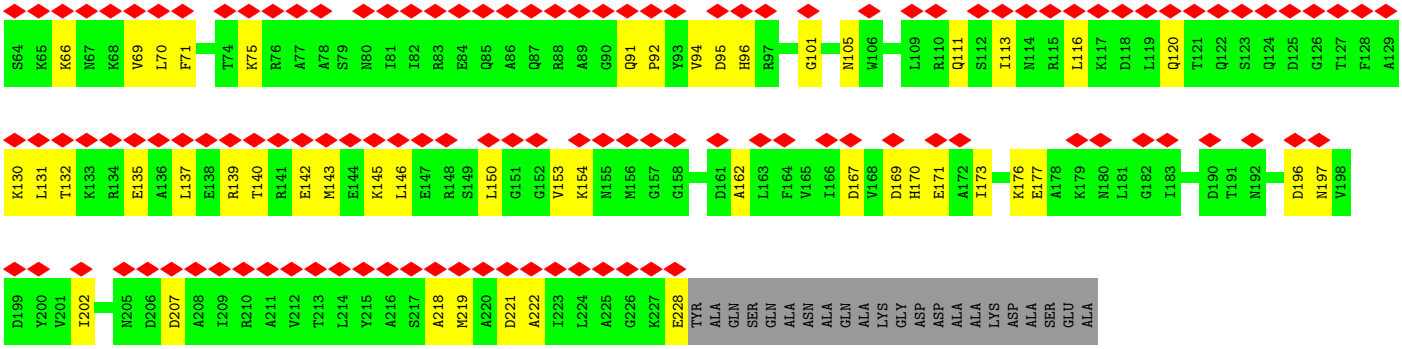


• Molecule 32: 30S ribosomal protein S2

Chain b:



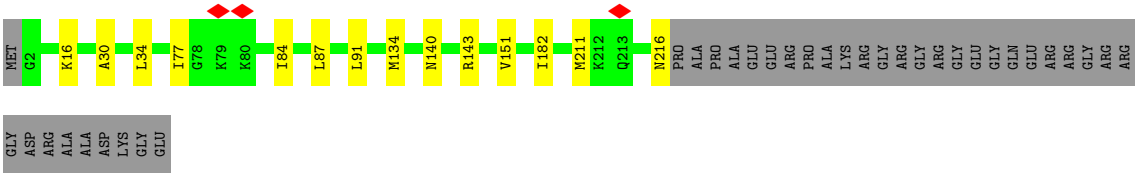




• Molecule 33: 30S ribosomal protein S3

Chain c:

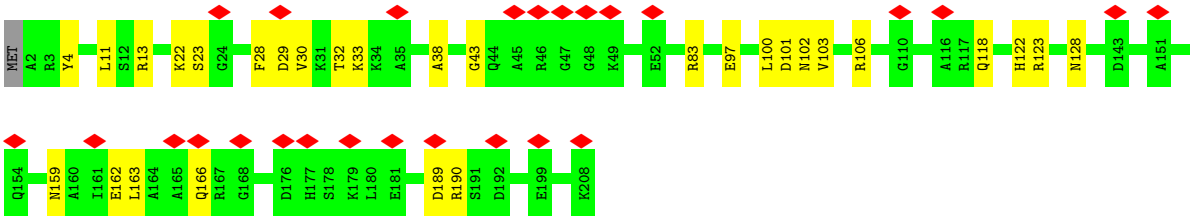




• Molecule 34: 30S ribosomal protein S4

Chain d:

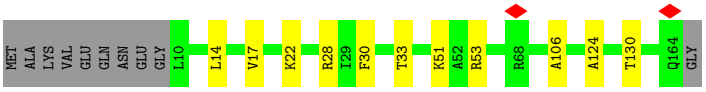




• Molecule 35: 30S ribosomal protein S5

Chain e:

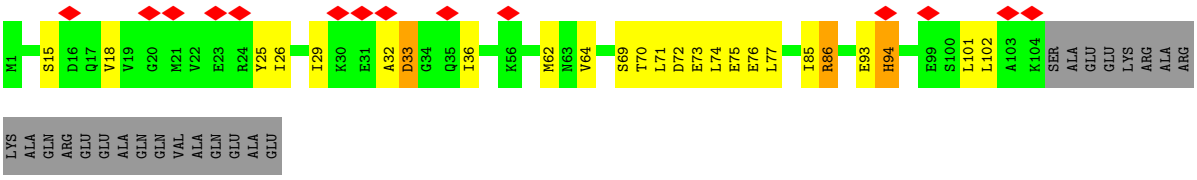




• Molecule 36: 30S ribosomal protein S6

Chain f:

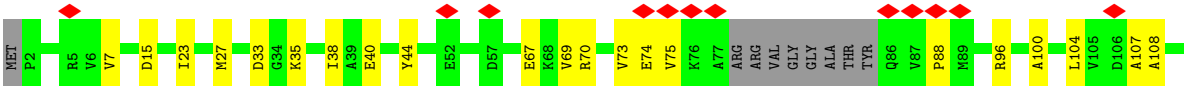


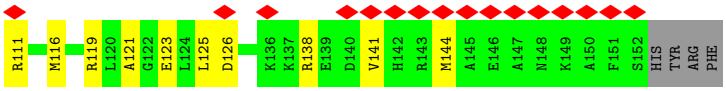


• Molecule 37: 30S ribosomal protein S7

Chain g:

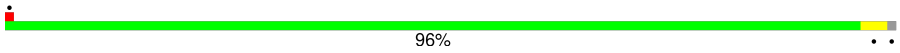


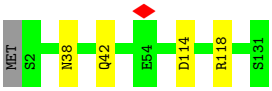




• Molecule 38: 30S ribosomal protein S8

Chain h:

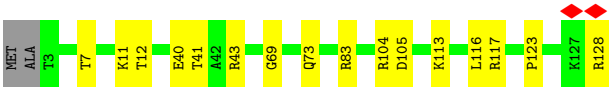




• Molecule 39: 30S ribosomal protein S9

Chain i:

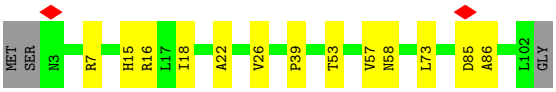




• Molecule 40: 30S ribosomal protein S10

Chain j:

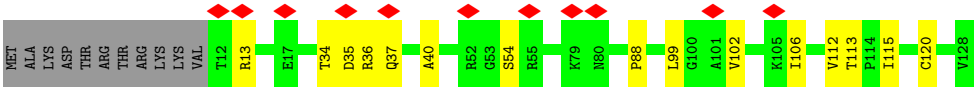




• Molecule 41: 30S ribosomal protein S11

Chain k:

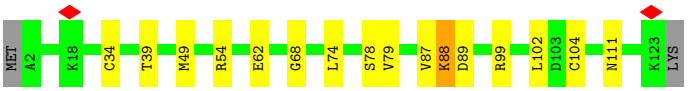




• Molecule 42: 30S ribosomal protein S12

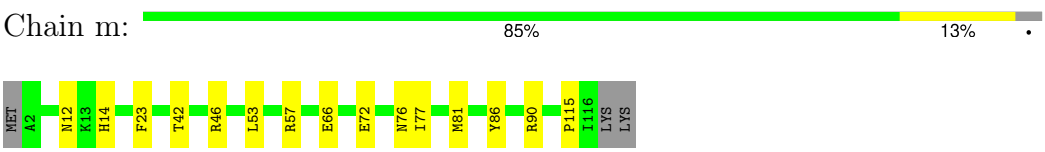
Chain l:





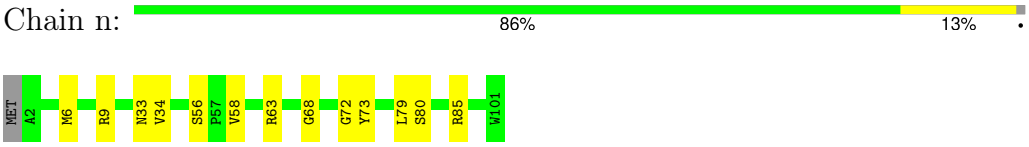
• Molecule 43: 30S ribosomal protein S13

Chain m:



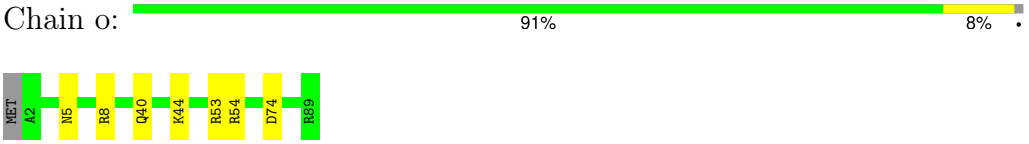
• Molecule 44: 30S ribosomal protein S14

Chain n:



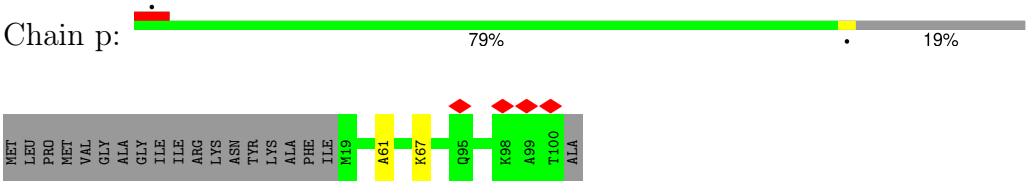
• Molecule 45: 30S ribosomal protein S15

Chain o:



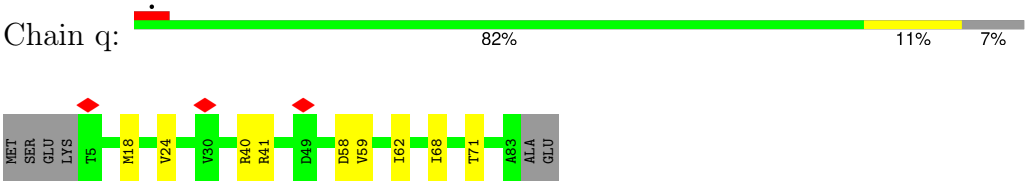
• Molecule 46: 30S ribosomal protein S16

Chain p:



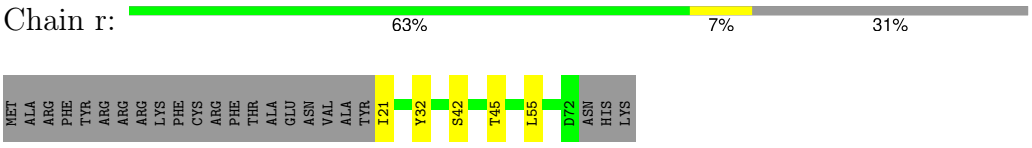
• Molecule 47: 30S ribosomal protein S17

Chain q:



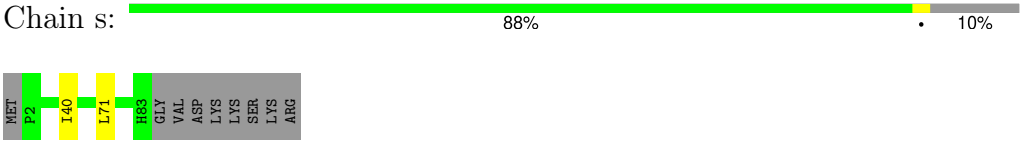
• Molecule 48: 30S ribosomal protein S18

Chain r:



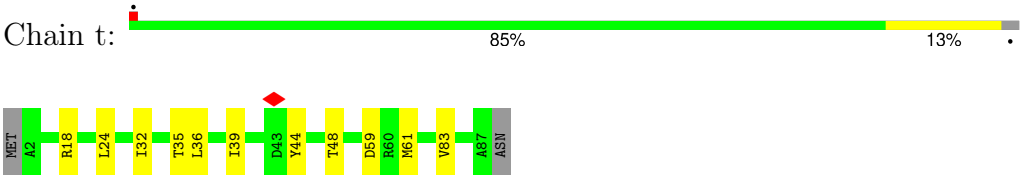
• Molecule 49: 30S ribosomal protein S19

Chain s:



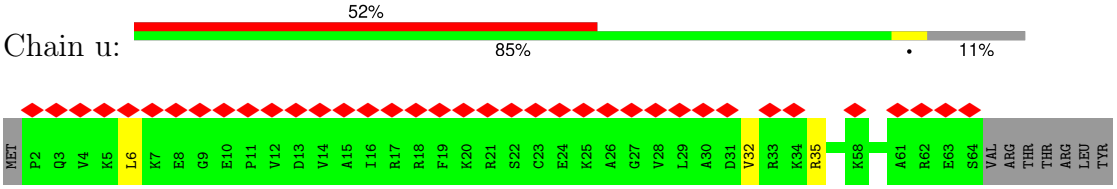
• Molecule 50: 30S ribosomal protein S20

Chain t:



• Molecule 51: 30S ribosomal protein S21

Chain u:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79574	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.918	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	434.176, 434.176, 434.176	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MC, 2MG, 4OC, PSU, 6MZ, OMU, 2MA, YQM, G7M, MA6, 5MU, 3TD, OMG, ZN, UR3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.13	0/434	0.26	0/573
2	1	0.14	0/367	0.28	0/481
3	2	0.15	0/515	0.41	0/678
4	3	0.20	0/296	0.40	0/389
5	A	0.10	0/65229	0.26	0/101736
6	B	0.10	0/2739	0.28	0/4266
7	C	0.13	0/2152	0.35	0/2891
8	D	0.11	0/1590	0.28	0/2142
9	E	0.11	0/1537	0.28	0/2073
10	F	0.17	0/1390	0.45	0/1863
11	G	0.11	0/1337	0.30	0/1807
12	H	0.13	0/461	0.33	0/616
13	I	0.12	0/1151	0.28	0/1551
14	J	0.12	0/956	0.30	0/1286
15	K	0.10	0/1079	0.28	0/1439
16	L	0.13	0/1104	0.29	0/1475
17	M	0.14	0/956	0.33	0/1282
18	N	0.09	0/865	0.24	0/1156
19	O	0.12	0/925	0.32	0/1241
20	P	0.14	0/947	0.30	0/1262
21	Q	0.12	0/818	0.30	0/1094
22	R	0.13	0/831	0.26	0/1113
23	S	0.11	0/716	0.25	0/957
24	T	0.08	0/770	0.24	0/1034
25	U	0.11	0/770	0.29	0/1036
26	V	0.10	0/593	0.28	0/793
27	W	0.09	0/642	0.26	0/856
28	X	0.11	0/487	0.23	0/646
29	Y	0.10	0/460	0.25	0/614
30	Z	0.09	0/462	0.24	0/615
31	a	0.12	0/36476	0.27	0/56895
32	b	0.17	0/1799	0.39	0/2429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.13	0/1714	0.31	0/2304
34	d	0.12	0/1653	0.32	0/2213
35	e	0.13	0/1141	0.32	0/1537
36	f	0.14	0/882	0.38	0/1189
37	g	0.15	0/1142	0.33	0/1528
38	h	0.11	0/993	0.29	0/1331
39	i	0.19	0/1002	0.36	0/1339
40	j	0.14	0/811	0.33	0/1096
41	k	0.13	0/878	0.31	0/1189
42	l	0.14	0/958	0.40	0/1284
43	m	0.29	1/913 (0.1%)	0.55	3/1226 (0.2%)
44	n	0.15	0/803	0.34	0/1071
45	o	0.13	0/715	0.31	0/958
46	p	0.11	0/655	0.33	0/879
47	q	0.12	0/628	0.33	0/847
48	r	0.11	0/432	0.29	0/583
49	s	0.13	0/664	0.30	0/897
50	t	0.16	0/669	0.28	0/892
51	u	0.10	0/528	0.23	0/697
All	All	0.11	1/148035 (0.0%)	0.28	3/221349 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	m	115	PRO	CG-CD	-6.81	1.27	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	m	115	PRO	N-CD-CG	-9.97	88.24	103.20
43	m	115	PRO	CA-N-CD	-7.31	101.77	112.00
43	m	115	PRO	CA-CB-CG	-5.22	94.58	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	427	0	462	2	0
2	1	363	0	401	1	0
3	2	509	0	566	6	0
4	3	295	0	326	4	0
5	A	58566	0	29451	223	0
6	B	2450	0	1241	16	0
7	C	2111	0	2176	19	0
8	D	1572	0	1610	11	0
9	E	1516	0	1569	9	0
10	F	1370	0	1420	44	0
11	G	1318	0	1373	15	0
12	H	458	0	480	4	0
13	I	1125	0	1148	4	0
14	J	946	0	1007	2	0
15	K	1071	0	1140	3	0
16	L	1087	0	1162	13	0
17	M	942	0	987	3	0
18	N	857	0	899	4	0
19	O	913	0	968	6	0
20	P	934	0	997	3	0
21	Q	807	0	842	5	0
22	R	826	0	894	2	0
23	S	710	0	768	5	0
24	T	766	0	816	7	0
25	U	760	0	783	4	0
26	V	585	0	589	1	0
27	W	632	0	667	0	0
28	X	486	0	528	1	0
29	Y	455	0	476	3	0
30	Z	456	0	448	3	0
31	a	32782	0	16507	135	0
32	b	1769	0	1787	43	0
33	c	1690	0	1774	8	0
34	d	1631	0	1691	19	0
35	e	1129	0	1174	7	0
36	f	867	0	868	21	0
37	g	1127	0	1176	27	0
38	h	985	0	1047	2	0
39	i	991	0	1048	11	0
40	j	801	0	832	10	0
41	k	862	0	877	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	l	945	0	998	12	0
43	m	903	0	962	7	0
44	n	792	0	833	7	0
45	o	705	0	712	5	0
46	p	644	0	655	1	0
47	q	621	0	665	7	0
48	r	426	0	447	3	0
49	s	646	0	663	1	0
50	t	663	0	715	7	0
51	u	522	0	565	5	0
52	3	1	0	0	0	0
53	A	80	0	0	0	0
53	a	40	0	0	0	0
54	A	136	0	0	0	0
54	B	1	0	0	0	0
54	D	1	0	0	0	0
54	K	1	0	0	0	0
54	a	52	0	0	0	0
55	2	2	0	0	0	0
55	A	597	0	0	25	0
55	B	4	0	0	0	0
55	C	7	0	0	0	0
55	D	4	0	0	0	0
55	E	3	0	0	0	0
55	K	7	0	0	0	0
55	R	1	0	0	0	0
55	U	1	0	0	0	0
55	Z	2	0	0	1	0
55	a	156	0	0	12	0
55	i	2	0	0	0	0
55	j	3	0	0	0	0
55	k	1	0	0	0	0
55	m	1	0	0	0	0
55	n	3	0	0	0	0
55	q	1	0	0	0	0
55	s	1	0	0	0	0
55	t	1	0	0	0	0
All	All	137923	0	92190	706	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (706) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:85:G:O2'	31:a:86:C:OP2	1.76	1.01
10:F:17:GLN:NE2	10:F:22:ILE:O	1.95	0.99
31:a:789:A:O2'	31:a:790:U:OP2	1.81	0.99
10:F:7:ARG:NH2	10:F:11:GLU:OE1	1.99	0.95
31:a:1490:A:O2'	31:a:1491:G:N7	2.03	0.91
5:A:799:G:O2'	5:A:800:A:OP1	1.86	0.91
5:A:1843:A:O2'	5:A:1844:A:N7	2.06	0.89
43:m:12:ASN:OD1	43:m:46:ARG:NH2	2.06	0.87
42:l:34:CYS:HG	42:l:78:SER:HG	1.22	0.86
31:a:423:U:OP2	31:a:424:G:O2'	1.94	0.86
5:A:1865:G:N2	5:A:1868:A:OP2	2.10	0.85
6:B:55:A:O2'	10:F:27:GLU:OE2	1.94	0.84
5:A:849:C:OP1	29:Y:49:LYS:NZ	2.11	0.84
5:A:2631:U:O2'	8:D:82:GLU:OE2	1.94	0.84
5:A:324:A:O2'	5:A:325:G:OP1	1.93	0.84
38:h:38:ASN:O	38:h:42:GLN:NE2	2.11	0.83
5:A:184:G:OP2	5:A:184:G:N2	2.13	0.82
5:A:1230:G:O2'	5:A:1231:G:O4'	1.98	0.82
5:A:533:U:O2'	20:P:49:ASP:OD2	1.97	0.82
33:c:140:ASN:OD1	33:c:143:ARG:NH2	2.12	0.81
39:i:104:ARG:NH1	39:i:105:ASP:O	2.14	0.81
24:T:28:SER:OG	24:T:29:GLU:OE1	1.97	0.81
5:A:2861:U:OP2	5:A:2862:G:O2'	1.99	0.81
5:A:616:G:O6	55:A:3401:HOH:O	1.98	0.80
5:A:2311:C:O2	10:F:125:ARG:NH2	2.15	0.80
31:a:572:G:O2'	31:a:818:G:OP2	1.98	0.79
5:A:2097:A:N6	5:A:2184:U:O4	2.16	0.79
5:A:364:A:OP2	5:A:424:G:O2'	2.02	0.78
5:A:1306:G:OP2	5:A:1306:G:N2	2.13	0.77
31:a:728:G:OP2	55:a:1703:HOH:O	2.04	0.76
31:a:936:G:O6	55:a:1701:HOH:O	2.01	0.76
5:A:1016:U:OP1	5:A:1032:U:O2'	2.03	0.76
5:A:789:C:OP2	55:A:3403:HOH:O	2.02	0.75
42:l:54:ARG:NH1	42:l:62:GLU:OE2	2.19	0.75
31:a:949:U:OP2	55:a:1702:HOH:O	2.02	0.75
35:e:33:THR:HG22	35:e:51:LYS:HG2	1.69	0.75
40:j:85:ASP:OD1	40:j:86:ALA:N	2.20	0.75
5:A:226:A:N3	5:A:241:U:O2'	2.20	0.75
10:F:34:ILE:HD13	10:F:156:ILE:HG22	1.69	0.75
5:A:1327:G:OP2	55:A:3404:HOH:O	2.04	0.75
31:a:604:A:OP1	55:a:1704:HOH:O	2.05	0.75
36:f:26:ILE:HD12	36:f:36:ILE:HD13	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1749:G:N2	5:A:1752:G:OP2	2.18	0.75
5:A:1938:C:OP2	5:A:1939:U:O2'	2.02	0.75
5:A:1323:A:OP2	55:A:3405:HOH:O	2.05	0.74
5:A:1183:U:OP1	55:A:3407:HOH:O	2.05	0.73
5:A:787:A:OP1	55:A:3409:HOH:O	2.06	0.73
10:F:34:ILE:CD1	10:F:156:ILE:HG22	2.19	0.73
5:A:1348:A:O3'	7:C:38:LYS:NZ	2.22	0.72
31:a:789:A:HO2'	31:a:790:U:P	2.11	0.72
31:a:545:G:OP1	55:a:1705:HOH:O	2.07	0.72
5:A:527:A:OP1	55:A:3408:HOH:O	2.06	0.72
5:A:2064:U:OP2	55:A:3406:HOH:O	2.05	0.72
31:a:1049:U:OP2	55:a:1706:HOH:O	2.08	0.72
42:l:39:THR:HG21	42:l:49:MET:HE2	1.71	0.72
5:A:788:U:OP2	55:A:3409:HOH:O	2.08	0.72
5:A:2709:C:OP2	55:A:3410:HOH:O	2.09	0.71
44:n:56:SER:OG	44:n:58:VAL:HG12	1.91	0.71
5:A:363:G:OP2	5:A:364:A:O2'	2.02	0.71
5:A:809:U:OP1	55:A:3411:HOH:O	2.09	0.71
41:k:34:THR:HG22	41:k:40:ALA:HA	1.72	0.70
5:A:1937:C:N4	5:A:1961:C:O4'	2.23	0.70
31:a:349:A:OP2	55:a:1708:HOH:O	2.09	0.70
31:a:174:C:OP2	55:a:1707:HOH:O	2.08	0.70
31:a:1429:G:O2'	31:a:1465:A:N6	2.25	0.70
5:A:2465:A:N6	5:A:2477:G:O2'	2.25	0.70
5:A:2294:A:OP1	10:F:71:ARG:NE	2.24	0.69
5:A:2508:C:OP2	8:D:131:ARG:NH2	2.25	0.69
31:a:1347:A:O2'	37:g:33:ASP:OD1	2.11	0.69
3:2:33:THR:OG1	5:A:2416:C:OP1	2.08	0.69
19:O:40:ARG:NH1	31:a:341:C:OP1	2.26	0.68
23:S:5:ARG:O	23:S:9:VAL:HG23	1.93	0.68
31:a:1120:A:O2'	40:j:39:PRO:O	2.10	0.68
39:i:117:ARG:NH1	39:i:123:PRO:HA	2.09	0.68
37:g:67:GLU:OE1	37:g:70:ARG:NH1	2.26	0.68
43:m:77:ILE:HG22	43:m:81:MET:HE2	1.76	0.68
5:A:2577:G:OP2	5:A:2577:G:N2	2.26	0.68
31:a:351:C:OP2	55:a:1710:HOH:O	2.12	0.68
5:A:378:G:N7	55:A:3432:HOH:O	2.27	0.67
5:A:572:A:OP1	55:A:3415:HOH:O	2.13	0.67
31:a:1123:U:O2'	31:a:1124:G:OP1	2.11	0.67
31:a:1074:G:N2	31:a:1077:A:OP2	2.23	0.67
16:L:48:GLU:OE2	16:L:51:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:207:G:O2'	31:a:208:G:O4'	2.13	0.67
5:A:941:C:OP2	55:A:3414:HOH:O	2.12	0.67
13:I:23:LYS:NZ	13:I:142:ILE:O	2.29	0.66
31:a:85:G:HO2'	31:a:86:C:P	2.14	0.66
5:A:978:A:OP2	5:A:979:C:N4	2.29	0.66
31:a:691:A:OP1	41:k:54:SER:OG	2.07	0.65
5:A:1292:C:OP2	55:A:3416:HOH:O	2.14	0.65
41:k:106:ILE:O	51:u:6:LEU:HD12	1.96	0.65
11:G:104:ASN:ND2	11:G:114:ASP:OD1	2.28	0.65
5:A:962:C:OP2	55:A:3417:HOH:O	2.14	0.65
33:c:216:ASN:OD1	40:j:16:ARG:NE	2.29	0.65
5:A:1413:G:N2	5:A:1577:A:N7	2.45	0.65
41:k:113:THR:HG21	51:u:32:VAL:HG21	1.80	0.65
6:B:43:A:O4'	10:F:92:ARG:NH1	2.29	0.64
39:i:117:ARG:HH12	39:i:123:PRO:HA	1.62	0.64
5:A:2687:C:HO2'	5:A:2867:U:HO2'	1.45	0.64
32:b:221:ASP:OD1	32:b:222:ALA:N	2.30	0.64
5:A:1822:G:H5"	7:C:223:MET:HE2	1.79	0.64
5:A:2591:G:N2	5:A:2594:A:OP2	2.24	0.64
2:1:29:GLN:NE2	5:A:217:C:OP1	2.30	0.64
6:B:38:U:O2'	6:B:41:C:OP2	2.06	0.64
11:G:13:ASN:OD1	11:G:14:GLY:N	2.30	0.64
31:a:813:A:OP2	55:a:1711:HOH:O	2.15	0.64
32:b:116:LEU:HD13	32:b:146:LEU:HB3	1.80	0.64
5:A:2219:G:OP1	7:C:171:TYR:OH	2.12	0.64
31:a:1230:G:OP1	39:i:117:ARG:NH2	2.29	0.63
31:a:755:G:O6	55:a:1709:HOH:O	2.11	0.63
5:A:1198:U:OP2	5:A:1199:A:O2'	2.05	0.63
5:A:1810:G:OP2	5:A:1811:A:O2'	2.08	0.63
31:a:1446:U:HO2'	31:a:1447:G:P	2.22	0.63
36:f:26:ILE:CD1	36:f:36:ILE:HD13	2.28	0.63
19:O:23:PHE:O	19:O:53:LYS:NZ	2.30	0.63
5:A:2379:G:O2'	5:A:2380:U:OP1	2.15	0.63
31:a:1446:U:O2'	31:a:1447:G:O5'	2.15	0.62
5:A:69:U:O4	5:A:70:A:N6	2.33	0.62
41:k:120:CYS:O	51:u:35:ARG:NH2	2.33	0.62
23:S:1:MET:HE3	23:S:41:GLU:HG2	1.82	0.62
31:a:610:C:OP1	34:d:83:ARG:NH1	2.29	0.62
50:t:24:LEU:HD22	50:t:61:MET:HE1	1.81	0.62
5:A:2844:G:O2'	5:A:2864:A:N6	2.32	0.61
31:a:6:C:H42	31:a:610:C:H5"	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:508:C:O2'	31:a:509:U:OP2	2.16	0.61
34:d:101:ASP:OD1	34:d:102:ASN:N	2.33	0.61
31:a:1124:G:OP1	31:a:1277:A:O2'	2.18	0.61
5:A:2309:C:O4'	10:F:37:ASN:ND2	2.34	0.61
31:a:1010:G:N2	31:a:1013:A:OP2	2.26	0.61
5:A:2518:U:O2'	5:A:2643:U:OP1	2.15	0.60
31:a:603:G:N2	31:a:629:U:OP1	2.33	0.60
5:A:829:G:OP2	55:A:3420:HOH:O	2.16	0.60
5:A:2568:A:O2'	5:A:2571:C:OP1	2.15	0.60
6:B:12:U:O3'	6:B:104:U:O2'	2.20	0.60
5:A:1962:A:N3	5:A:2588:G:O2'	2.32	0.60
44:n:63:ARG:NH1	44:n:68:GLY:O	2.31	0.60
31:a:808:C:O2'	31:a:898:A:N1	2.34	0.59
31:a:249:U:O2'	47:q:18:MET:SD	2.54	0.59
20:P:107:ALA:O	20:P:111:GLU:OE1	2.20	0.59
31:a:649:U:O4	31:a:749:G:O2'	2.16	0.59
6:B:12:U:OP2	6:B:68:C:O2'	2.19	0.59
32:b:70:LEU:HD21	32:b:94:VAL:HG23	1.84	0.58
32:b:169:ASP:OD1	32:b:170:HIS:N	2.35	0.58
10:F:101:ASP:OD2	10:F:102:ARG:N	2.36	0.58
31:a:316:G:O2'	31:a:1432:G:O2'	2.19	0.58
34:d:4:TYR:CE2	34:d:11:LEU:HD11	2.39	0.58
48:r:32:TYR:CD1	48:r:55:LEU:HD11	2.38	0.58
5:A:1909:A:H62	31:a:1406:C:H1'	1.68	0.58
10:F:79:ILE:HD13	10:F:85:ILE:HD13	1.85	0.58
5:A:2721:A:O2'	5:A:2722:U:OP2	2.19	0.58
32:b:57:ASN:O	32:b:61:GLN:OE1	2.21	0.58
31:a:405:U:OP1	34:d:23:SER:OG	2.21	0.58
15:K:112:ILE:HB	15:K:129:LEU:HD23	1.86	0.58
31:a:122:A:OP1	31:a:602:U:O2'	2.20	0.58
5:A:1452:U:O4	55:A:3421:HOH:O	2.16	0.57
16:L:79:LEU:HD23	16:L:80:GLU:HG3	1.86	0.57
5:A:2071:U:OP2	5:A:2234:G:O2'	2.22	0.57
34:d:162:GLU:O	34:d:166:GLN:OE1	2.23	0.57
36:f:26:ILE:HG23	36:f:36:ILE:CD1	2.34	0.57
10:F:123:ASP:O	10:F:125:ARG:NH1	2.38	0.57
31:a:964:5MC:H4'	39:i:128:ARG:HH12	1.69	0.57
31:a:1298:U:O2'	31:a:1299:C:H3'	2.05	0.57
24:T:5:LYS:O	24:T:24:VAL:HG11	2.04	0.57
31:a:809:G:H1'	31:a:810:U:OP2	2.04	0.57
32:b:52:LEU:O	32:b:56:LEU:HD23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:f:25:TYR:HE1	36:f:77:LEU:HD23	1.70	0.57
5:A:1044:G:O2'	5:A:1108:A:N6	2.38	0.56
10:F:137:VAL:HG23	10:F:137:VAL:O	2.05	0.56
37:g:35:LYS:HE2	37:g:38:ILE:HD13	1.86	0.56
50:t:44:TYR:O	50:t:48:THR:HG23	2.05	0.56
31:a:155:G:O2'	31:a:157:A:N7	2.36	0.56
5:A:1771:U:OP1	55:A:3424:HOH:O	2.18	0.56
33:c:77:ILE:HA	33:c:84:ILE:HG23	1.87	0.56
31:a:1098:A:N6	32:b:177:GLU:OE2	2.38	0.56
45:o:5:ASN:OD1	45:o:8:ARG:NH2	2.38	0.56
10:F:94:ASP:OD2	10:F:95:GLN:N	2.39	0.56
5:A:1106:C:H2'	5:A:1107:G:C5	2.40	0.56
31:a:1433:U:OP1	50:t:18:ARG:NH2	2.39	0.56
8:D:139:ASN:ND2	8:D:142:SER:O	2.39	0.56
5:A:1933:A:H1'	5:A:1935:5MU:H72	1.86	0.55
48:r:42:SER:HA	48:r:45:THR:HG22	1.89	0.55
5:A:1310:C:O2'	5:A:1387:A:N3	2.36	0.55
31:a:670:A:H2'	31:a:671:G:C8	2.41	0.55
31:a:973:G:OP2	31:a:1355:U:O2'	2.24	0.55
31:a:1050:G:H4'	31:a:1051:C:H3'	1.88	0.55
32:b:66:LYS:NZ	32:b:228:GLU:O	2.37	0.55
31:a:6:C:N4	31:a:610:C:OP1	2.40	0.55
32:b:120:GLN:OE1	32:b:154:LYS:NZ	2.39	0.55
11:G:99:LYS:NZ	11:G:104:ASN:OD1	2.20	0.54
43:m:72:GLU:OE2	43:m:76:ASN:ND2	2.40	0.54
5:A:843:G:O2'	5:A:845:A:N7	2.41	0.54
16:L:33:ALA:HB2	16:L:105:GLU:HG2	1.89	0.54
32:b:196:ASP:OD1	32:b:197:ASN:N	2.40	0.54
24:T:6:LYS:O	24:T:24:VAL:HG13	2.07	0.54
31:a:562:U:OP2	31:a:563:G:O2'	2.25	0.54
5:A:308:U:H2'	5:A:309:G:O4'	2.08	0.54
8:D:18:ASP:OD1	8:D:19:ALA:N	2.40	0.54
31:a:1237:U:H5	37:g:116:MET:HE3	1.73	0.54
47:q:71:THR:O	47:q:71:THR:HG22	2.08	0.54
10:F:138:PHE:CG	10:F:139:PRO:HD3	2.43	0.54
5:A:2689:G:OP1	55:A:3423:HOH:O	2.18	0.53
42:l:39:THR:HG21	42:l:49:MET:HB2	1.88	0.53
33:c:16:LYS:NZ	33:c:182:ILE:O	2.40	0.53
10:F:106:ILE:HD12	10:F:138:PHE:CB	2.39	0.53
36:f:71:LEU:O	36:f:75:GLU:OE1	2.26	0.53
10:F:169:LEU:HD21	10:F:173:PHE:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:71:ARG:NH1	10:F:72:LYS:HG3	2.23	0.53
18:N:42:SER:OG	18:N:44:ASP:OD2	2.25	0.53
20:P:97:ASP:OD1	20:P:101:HIS:ND1	2.35	0.53
31:a:1123:U:O2'	31:a:1124:G:P	2.66	0.53
3:2:30:HIS:CE1	3:2:31:ILE:HG13	2.44	0.53
6:B:9:C:OP1	26:V:72:LYS:NZ	2.37	0.53
42:l:87:VAL:O	42:l:88:LYS:CB	2.57	0.53
9:E:105:GLN:NE2	9:E:199:LEU:O	2.41	0.52
12:H:5:LEU:HD22	12:H:9:ILE:HD13	1.91	0.52
16:L:57:ARG:HE	16:L:120:LEU:CD1	2.23	0.52
6:B:11:A:O2'	6:B:13:A:OP2	2.27	0.52
9:E:111:LEU:CD2	9:E:116:ARG:HE	2.22	0.52
5:A:2843:U:H2'	5:A:2844:G:O4'	2.10	0.52
31:a:917:U:O2'	31:a:1078:G:O2'	2.01	0.52
34:d:29:ASP:OD1	34:d:30:VAL:N	2.42	0.52
5:A:1267:A:O2'	5:A:1269:A:OP1	2.26	0.52
41:k:113:THR:O	41:k:115:ILE:HD12	2.09	0.52
31:a:710:G:H2'	31:a:711:G:C8	2.45	0.52
32:b:69:VAL:HG13	32:b:71:PHE:CE1	2.45	0.52
33:c:30:ALA:O	33:c:34:LEU:HD23	2.10	0.52
5:A:272:A:N1	5:A:426:U:O2'	2.40	0.52
5:A:1154:A:OP2	55:A:3422:HOH:O	2.18	0.52
5:A:2524:U:O2'	5:A:2526:A:OP1	2.26	0.52
32:b:49:VAL:HG23	32:b:50:PRO:HD3	1.92	0.52
40:j:57:VAL:HG23	40:j:57:VAL:O	2.10	0.52
5:A:2026:6MZ:O2'	5:A:2027:A:OP2	2.20	0.52
31:a:1123:U:OP1	40:j:7:ARG:NH1	2.41	0.52
5:A:627:A:N3	5:A:637:U:O2'	2.43	0.51
5:A:228:A:O4'	5:A:240:A:O2'	2.25	0.51
5:A:1320:U:OP1	5:A:1645:U:O2'	2.26	0.51
15:K:134:LYS:NZ	15:K:138:GLU:OE2	2.41	0.51
36:f:101:LEU:HD23	36:f:102:LEU:HG	1.92	0.51
41:k:112:VAL:HG12	41:k:112:VAL:O	2.11	0.51
5:A:92:G:C2	5:A:106:U:O2	2.63	0.51
5:A:2056:A:O2'	5:A:2057:G:OP2	2.27	0.51
9:E:14:SER:N	9:E:196:GLU:OE1	2.43	0.51
14:J:75:SER:OG	19:O:76:VAL:O	2.18	0.51
5:A:2295:G:OP1	10:F:72:LYS:NZ	2.44	0.51
5:A:2379:G:O2'	5:A:2380:U:P	2.69	0.51
42:l:68:GLY:O	42:l:99:ARG:NH1	2.43	0.51
5:A:570:A:OP2	21:Q:80:ARG:NH1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:43:LEU:HD11	11:G:50:LEU:HD22	1.90	0.51
31:a:1263:G:N2	31:a:1266:A:OP2	2.42	0.51
32:b:75:LYS:NZ	32:b:207:ASP:OD1	2.31	0.51
35:e:130:THR:HG22	35:e:130:THR:O	2.11	0.51
44:n:6:MET:SD	44:n:9:ARG:NH2	2.83	0.51
11:G:89:LEU:HG	11:G:162:VAL:HG22	1.93	0.51
32:b:153:VAL:O	32:b:153:VAL:HG22	2.11	0.51
5:A:1812:C:N4	7:C:35:GLU:OE2	2.32	0.51
18:N:63:THR:O	18:N:64:THR:OG1	2.23	0.51
31:a:242:A:C2	31:a:278:A:C5	2.98	0.51
40:j:53:THR:HG22	44:n:85:ARG:HE	1.75	0.51
5:A:1793:C:HO2'	7:C:257:THR:HG1	1.59	0.51
5:A:1833:C:O2'	5:A:1923:A:N3	2.42	0.51
8:D:86:THR:HG22	8:D:87:GLU:N	2.26	0.51
37:g:69:VAL:HG11	37:g:104:LEU:HD11	1.92	0.51
31:a:426:A:OP2	34:d:22:LYS:NZ	2.40	0.50
32:b:95:ASP:OD1	32:b:96:HIS:N	2.44	0.50
10:F:31:ILE:HG23	10:F:31:ILE:O	2.11	0.50
31:a:425:U:O2'	34:d:22:LYS:NZ	2.41	0.50
32:b:218:ALA:O	32:b:221:ASP:OD1	2.29	0.50
5:A:1717:G:O2'	5:A:1735:A:N6	2.45	0.50
5:A:2294:A:OP1	10:F:71:ARG:NH2	2.44	0.50
6:B:11:A:O4'	6:B:13:A:O2'	2.29	0.50
32:b:132:THR:HG23	32:b:135:GLU:H	1.75	0.50
5:A:97:C:OP2	5:A:98:A:O2'	2.23	0.50
31:a:1353:G:H2'	31:a:1354:A:C8	2.47	0.50
41:k:13:ARG:NH2	41:k:35:ASP:OD2	2.44	0.50
9:E:191:ALA:O	9:E:195:ILE:HG13	2.11	0.50
31:a:402:G:H21	34:d:118:GLN:HE22	1.60	0.50
34:d:28:PHE:O	34:d:32:THR:HG22	2.12	0.50
11:G:101:THR:O	11:G:101:THR:HG22	2.11	0.50
31:a:320:G:N1	31:a:323:A:OP2	2.43	0.50
5:A:1025:A:N3	5:A:2482:C:O2'	2.39	0.49
4:3:19:ARG:O	4:3:20:ASN:OD1	2.30	0.49
5:A:2830:G:H2'	5:A:2875:A:H61	1.77	0.49
5:A:805:U:OP2	15:K:43:ARG:NH2	2.46	0.49
5:A:2048:A:H4'	8:D:151:GLN:O	2.11	0.49
7:C:269:ARG:HD2	7:C:270:ASP:O	2.12	0.49
32:b:46:GLU:N	32:b:46:GLU:OE1	2.46	0.49
32:b:202:ILE:HG13	32:b:202:ILE:O	2.11	0.49
35:e:14:LEU:HD21	35:e:17:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:799:G:C2'	5:A:800:A:OP1	2.60	0.49
10:F:34:ILE:HD11	10:F:154:ILE:HG22	1.94	0.49
32:b:58:PHE:O	32:b:62:LEU:HD13	2.12	0.49
8:D:30:VAL:O	8:D:188:SER:OG	2.25	0.49
21:Q:51:ALA:HB3	21:Q:52:PRO:HD3	1.95	0.49
29:Y:39:ASP:OD1	29:Y:44:ARG:NE	2.45	0.49
5:A:2470:U:H2'	5:A:2470:U:O2	2.12	0.49
31:a:276:C:O4'	47:q:41:ARG:NH1	2.46	0.49
32:b:137:LEU:HA	32:b:140:THR:OG1	2.12	0.49
5:A:1373:A:O2'	5:A:1374:U:OP2	2.20	0.49
25:U:69:VAL:HG13	25:U:69:VAL:O	2.12	0.49
37:g:23:ILE:O	37:g:27:MET:HG3	2.12	0.49
48:r:21:ILE:HG23	48:r:21:ILE:O	2.12	0.49
5:A:72:C:O2'	5:A:455:C:N3	2.46	0.48
8:D:141:VAL:HG23	8:D:141:VAL:O	2.13	0.48
12:H:5:LEU:HD22	12:H:9:ILE:CD1	2.43	0.48
37:g:75:VAL:HG21	37:g:144:MET:CE	2.43	0.48
5:A:2287:U:H2'	5:A:2288:G:C8	2.48	0.48
32:b:69:VAL:HG23	32:b:162:ALA:HB3	1.94	0.48
35:e:30:PHE:O	35:e:53:ARG:NH1	2.46	0.48
37:g:111:ARG:NH2	37:g:126:ASP:OD2	2.46	0.48
39:i:69:GLY:O	39:i:73:GLN:HG3	2.13	0.48
50:t:32:ILE:O	50:t:35:THR:HG22	2.14	0.48
5:A:92:G:N1	5:A:106:U:C2	2.81	0.48
18:N:9:LEU:O	18:N:13:LYS:HG2	2.13	0.48
32:b:91:GLN:OE1	32:b:92:PRO:HD2	2.14	0.48
36:f:72:ASP:OD1	36:f:73:GLU:N	2.47	0.48
5:A:252:G:O2'	5:A:383:A:N1	2.39	0.48
5:A:782:G:C2	7:C:228:ILE:HD13	2.49	0.48
5:A:1950:G:O2'	5:A:1952:U:O4	2.23	0.48
16:L:6:ARG:HE	16:L:7:THR:H	1.60	0.48
32:b:7:SER:O	32:b:8:MET:HB2	2.14	0.48
32:b:173:ILE:O	32:b:177:GLU:OE1	2.32	0.48
34:d:32:THR:HG23	34:d:33:LYS:N	2.27	0.48
36:f:69:SER:O	36:f:70:THR:C	2.54	0.48
36:f:69:SER:O	36:f:72:ASP:OD1	2.32	0.48
50:t:39:ILE:HD11	50:t:83:VAL:HG23	1.95	0.48
5:A:2324:A:H2'	5:A:2325:A:C8	2.49	0.48
11:G:89:LEU:HD23	11:G:107:LEU:HD21	1.96	0.48
36:f:101:LEU:HD23	36:f:102:LEU:N	2.28	0.48
5:A:1854:A:N6	5:A:1880:G:O2'	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:122:ALA:O	7:C:130:LEU:HD21	2.14	0.48
19:O:35:VAL:HG21	19:O:44:GLN:CD	2.39	0.48
37:g:107:ALA:HB3	37:g:123:GLU:OE2	2.14	0.48
5:A:1517:G:OP2	5:A:1518:A:O2'	2.16	0.47
32:b:130:LYS:C	32:b:131:LEU:HD12	2.39	0.47
39:i:7:THR:O	39:i:83:ARG:HD2	2.13	0.47
5:A:313:A:H1'	5:A:314:G:OP1	2.15	0.47
5:A:1924:A:H2'	5:A:1925:G:O4'	2.13	0.47
31:a:397:C:O2'	31:a:618:A:N3	2.44	0.47
31:a:1394:C:OP2	35:e:28:ARG:NH2	2.47	0.47
34:d:97:GLU:OE2	34:d:106:ARG:NE	2.39	0.47
5:A:546:G:N3	5:A:546:G:H2'	2.29	0.47
34:d:189:ASP:OD1	34:d:190:ARG:N	2.46	0.47
37:g:108:ALA:O	37:g:119:ARG:NH1	2.48	0.47
47:q:58:ASP:OD1	47:q:59:VAL:N	2.47	0.47
5:A:566:U:O2'	55:A:3419:HOH:O	2.16	0.47
5:A:1775:U:OP2	5:A:1780:A:N6	2.31	0.47
10:F:34:ILE:HG23	10:F:34:ILE:O	2.12	0.47
31:a:1431:A:H2'	31:a:1432:G:O4'	2.14	0.47
33:c:87:LEU:O	33:c:91:LEU:HD13	2.14	0.47
3:2:30:HIS:ND1	3:2:31:ILE:HG13	2.28	0.47
5:A:391:C:C2	5:A:392:C:C5	3.02	0.47
5:A:1335:U:O2'	23:S:60:THR:OG1	2.22	0.47
11:G:80:SER:O	11:G:81:GLU:HB2	2.15	0.47
6:B:42:G:O2'	6:B:45:C:N4	2.47	0.47
31:a:180:U:C2	31:a:181:C:C5	3.03	0.47
31:a:367:A:H2'	31:a:368:C:O4'	2.15	0.47
43:m:14:HIS:ND1	43:m:42:THR:O	2.43	0.47
5:A:1542:A:O2'	5:A:1543:A:O4'	2.33	0.47
19:O:91:ARG:NH1	19:O:113:ILE:O	2.48	0.47
36:f:76:GLU:OE2	36:f:77:LEU:HD12	2.14	0.47
36:f:93:GLU:O	36:f:94:HIS:CG	2.68	0.47
42:l:89:ASP:C	42:l:89:ASP:OD1	2.56	0.47
5:A:2610:A:OP1	55:A:3425:HOH:O	2.20	0.47
10:F:106:ILE:HD12	10:F:138:PHE:HB2	1.96	0.47
40:j:57:VAL:O	40:j:58:ASN:ND2	2.48	0.47
5:A:1343:C:C5	5:A:1344:C:C5	3.03	0.47
7:C:272:ARG:O	7:C:273:VAL:C	2.58	0.47
10:F:40:VAL:HG12	10:F:43:ALA:HB2	1.96	0.47
36:f:32:ALA:O	36:f:33:ASP:HB2	2.14	0.47
40:j:15:HIS:HA	40:j:18:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:799:G:HO2'	5:A:800:A:P	2.24	0.47
5:A:1421:G:OP2	5:A:1422:A:O2'	2.27	0.47
11:G:159:GLY:O	11:G:163:ARG:NH2	2.48	0.47
13:I:128:SER:OG	13:I:129:GLU:OE1	2.27	0.47
16:L:32:ILE:HD11	16:L:114:ALA:CB	2.45	0.47
5:A:1344:C:C2	5:A:1345:C:C5	3.04	0.46
37:g:75:VAL:HG21	37:g:144:MET:HE3	1.96	0.46
39:i:40:GLU:OE2	39:i:43:ARG:NH1	2.47	0.46
5:A:394:U:O2'	5:A:395:G:N7	2.48	0.46
31:a:1193:A:O2'	31:a:1194:A:OP1	2.28	0.46
31:a:1483:G:H2'	31:a:1484:G:O4'	2.15	0.46
5:A:713:A:N1	45:o:53:ARG:NH1	2.63	0.46
5:A:1347:U:O2'	5:A:1568:A:N3	2.45	0.46
5:A:2379:G:HO2'	5:A:2380:U:P	2.37	0.46
36:f:101:LEU:O	36:f:102:LEU:HB2	2.16	0.46
43:m:86:TYR:O	43:m:90:ARG:HG2	2.15	0.46
6:B:31:G:C2	6:B:48:A:C2	3.03	0.46
37:g:69:VAL:HG11	37:g:104:LEU:CD1	2.45	0.46
31:a:813:A:OP1	31:a:1523:G:O2'	2.28	0.46
31:a:1379:C:O2	31:a:1379:C:O4'	2.34	0.46
37:g:27:MET:CE	37:g:40:GLU:HG2	2.45	0.46
42:l:79:VAL:HG12	42:l:102:LEU:HD13	1.97	0.46
5:A:715:C:O2	5:A:715:C:O4'	2.34	0.46
5:A:1580:C:O2'	5:A:1583:C:N3	2.42	0.46
5:A:2548:OMU:OP2	5:A:2548:OMU:H6	2.16	0.46
17:M:19:ALA:O	17:M:23:ASN:ND2	2.48	0.46
31:a:1122:U:O2'	31:a:1123:U:H2'	2.16	0.46
37:g:69:VAL:HG12	37:g:69:VAL:O	2.15	0.46
5:A:1860:U:OP1	5:A:2406:G:O2'	2.33	0.46
6:B:30:U:C2	6:B:49:G:N2	2.84	0.46
31:a:607:U:N3	31:a:608:C:C5	2.83	0.46
34:d:100:LEU:O	34:d:103:VAL:HG22	2.16	0.46
10:F:141:ILE:HG22	10:F:142:ASP:N	2.31	0.46
16:L:111:GLU:O	16:L:115:ARG:HG3	2.16	0.46
31:a:1321:A:H2'	31:a:1322:C:O4'	2.16	0.46
32:b:142:GLU:O	32:b:146:LEU:HD13	2.15	0.46
5:A:1911:3TD:H10B	5:A:1912:A:H1'	1.98	0.46
21:Q:51:ALA:HB3	21:Q:52:PRO:CD	2.46	0.46
24:T:99:GLU:N	24:T:99:GLU:OE1	2.49	0.46
31:a:1123:U:H1'	31:a:1124:G:OP1	2.15	0.46
32:b:173:ILE:O	32:b:176:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:f:62:MET:HE2	36:f:64:VAL:HG11	1.97	0.46
46:p:61:ALA:HB3	46:p:67:LYS:HG2	1.96	0.46
50:t:32:ILE:O	50:t:36:LEU:HD13	2.15	0.46
8:D:110:VAL:HG11	8:D:180:ILE:HD11	1.98	0.46
24:T:34:VAL:HG11	24:T:37:LEU:HD12	1.98	0.46
5:A:1432:C:O2'	5:A:1512:G:O2'	2.31	0.45
31:a:1215:C:H2'	31:a:1216:A:C8	2.51	0.45
37:g:27:MET:HE3	37:g:40:GLU:HA	1.98	0.45
37:g:100:ALA:O	37:g:104:LEU:HD13	2.16	0.45
43:m:23:PHE:N	43:m:66:GLU:OE2	2.46	0.45
5:A:1548:U:OP1	5:A:1736:G:N2	2.50	0.45
31:a:555:G:OP1	55:a:1712:HOH:O	2.21	0.45
42:l:49:MET:O	42:l:49:MET:SD	2.74	0.45
25:U:38:ASN:C	25:U:38:ASN:OD1	2.59	0.45
32:b:167:ASP:OD1	32:b:167:ASP:N	2.49	0.45
34:d:159:ASN:O	34:d:163:LEU:HD23	2.16	0.45
47:q:40:ARG:O	47:q:41:ARG:NE	2.42	0.45
10:F:98:GLU:HA	10:F:101:ASP:OD1	2.17	0.45
11:G:71:VAL:O	11:G:75:LEU:HD13	2.16	0.45
31:a:1127:A:C8	31:a:1143:A:C2	3.04	0.45
25:U:4:PHE:CZ	25:U:59:VAL:HG23	2.52	0.45
31:a:711:G:H2'	31:a:712:A:C8	2.51	0.45
5:A:691:A:OP2	7:C:39:ARG:NH1	2.49	0.45
31:a:472:A:H2'	31:a:473:U:O4'	2.17	0.45
37:g:138:ARG:O	37:g:141:VAL:HG12	2.16	0.45
5:A:271:C:O2	5:A:271:C:O4'	2.34	0.45
5:A:324:A:C2'	5:A:325:G:OP1	2.65	0.45
5:A:1695:G:OP2	5:A:1696:A:O2'	2.31	0.45
7:C:183:LYS:NZ	7:C:266:MET:SD	2.90	0.45
16:L:78:PRO:O	16:L:79:LEU:HB2	2.17	0.45
31:a:515:C:O2	31:a:515:C:O4'	2.34	0.45
32:b:7:SER:O	32:b:49:VAL:HG11	2.16	0.45
3:2:7:ARG:NH1	5:A:258:A:OP1	2.50	0.45
5:A:1199:A:O4'	5:A:1201:G:C8	2.70	0.45
5:A:1634:G:H2'	5:A:1635:A:C8	2.51	0.45
10:F:91:LEU:HD12	10:F:95:GLN:CG	2.46	0.45
47:q:68:ILE:HG22	47:q:68:ILE:O	2.16	0.45
5:A:434:C:O2	5:A:434:C:O4'	2.34	0.45
5:A:847:A:H2'	5:A:848:C:C6	2.52	0.45
5:A:2282:G:H4'	5:A:2283:A:O4'	2.17	0.45
22:R:18:ARG:O	22:R:22:ASP:OD1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:101:GLY:O	32:b:105:ASN:N	2.42	0.45
34:d:22:LYS:O	34:d:23:SER:OG	2.33	0.45
5:A:392:C:C2	5:A:393:U:C5	3.05	0.44
5:A:1879:U:H2'	5:A:1880:G:C1'	2.46	0.44
31:a:682:G:H2'	31:a:683:U:C6	2.52	0.44
31:a:1051:C:H1'	31:a:1052:A:OP2	2.17	0.44
31:a:1180:C:O2'	31:a:1182:G:OP2	2.30	0.44
31:a:1374:A:C6	37:g:7:VAL:HG21	2.52	0.44
41:k:88:PRO:CG	51:u:32:VAL:HG11	2.47	0.44
30:Z:5:GLN:OE1	55:Z:101:HOH:O	2.21	0.44
49:s:40:ILE:HG13	49:s:71:LEU:HD22	1.99	0.44
5:A:2683:U:H2'	5:A:2684:G:O4'	2.16	0.44
10:F:28:ILE:HD12	10:F:28:ILE:H	1.82	0.44
10:F:170:MET:SD	10:F:175:PHE:HB3	2.58	0.44
36:f:15:SER:O	36:f:18:VAL:HG22	2.17	0.44
5:A:2502:U:OP2	5:A:2572:G:N1	2.50	0.44
7:C:167:ARG:HG2	7:C:172:ALA:HB2	1.98	0.44
31:a:1079:A:OP1	35:e:22:LYS:NZ	2.32	0.44
35:e:106:ALA:HB2	35:e:124:ALA:HB3	1.99	0.44
5:A:1317:A:C5	5:A:1318:C:C5	3.06	0.44
5:A:2633:U:H2'	5:A:2634:G:O4'	2.18	0.44
7:C:183:LYS:O	7:C:266:MET:HE3	2.17	0.44
21:Q:51:ALA:CB	21:Q:52:PRO:HD3	2.48	0.44
7:C:271:ARG:O	7:C:272:ARG:HB2	2.16	0.44
31:a:1073:C:H2'	31:a:1074:G:O4'	2.18	0.44
34:d:13:ARG:NH2	34:d:38:ALA:O	2.50	0.44
51:u:35:ARG:O	51:u:35:ARG:HG2	2.17	0.44
5:A:1816:U:H4'	5:A:1817:A:OP2	2.18	0.44
6:B:13:A:O3'	6:B:14:G:H8	2.01	0.44
22:R:63:SER:O	22:R:63:SER:OG	2.33	0.44
32:b:167:ASP:OD1	32:b:171:GLU:OE1	2.36	0.44
42:l:111:ASN:OD1	42:l:111:ASN:O	2.36	0.44
5:A:79:A:C8	28:X:54:LYS:HD2	2.53	0.44
5:A:390:A:C5	5:A:391:C:C5	3.06	0.44
10:F:81:ASP:C	10:F:81:ASP:OD1	2.61	0.44
16:L:63:LYS:HE3	16:L:65:PHE:CZ	2.53	0.44
37:g:73:VAL:HG12	37:g:74:GLU:N	2.33	0.44
5:A:509:C:N3	5:A:510:U:C5	2.86	0.44
5:A:1036:A:H2	5:A:1113:G:H22	1.64	0.44
31:a:143:G:H2'	31:a:144:G:C8	2.53	0.44
39:i:11:LYS:O	39:i:12:THR:OG1	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:36:ARG:O	41:k:37:GLN:HB2	2.17	0.44
5:A:2045:G:O6	55:A:3426:HOH:O	2.21	0.43
31:a:748:U:H2'	31:a:749:G:O4'	2.18	0.43
34:d:38:ALA:HB3	34:d:43:GLY:HA2	2.00	0.43
5:A:782:G:H5'	5:A:783:G:OP1	2.18	0.43
5:A:799:G:O2'	5:A:800:A:P	2.75	0.43
5:A:1469:U:H2'	5:A:1470:G:O4'	2.18	0.43
16:L:17:ASN:OD1	16:L:17:ASN:C	2.61	0.43
30:Z:53:LEU:O	30:Z:54:PHE:HB2	2.18	0.43
5:A:2067:A:H2'	5:A:2068:C:C6	2.53	0.43
10:F:7:ARG:CZ	10:F:11:GLU:OE1	2.65	0.43
32:b:145:LYS:HE3	32:b:146:LEU:HD12	2.00	0.43
5:A:591:U:H2'	5:A:592:U:C6	2.54	0.43
6:B:31:G:H2'	6:B:32:A:O4'	2.19	0.43
10:F:108:ILE:CG1	10:F:109:PRO:HD3	2.49	0.43
11:G:54:PRO:HB3	11:G:61:ALA:HB1	2.00	0.43
16:L:66:ILE:HD11	16:L:68:VAL:HG22	2.00	0.43
31:a:504:C:OP2	31:a:505:U:O2'	2.08	0.43
1:0:2:ARG:NH1	5:A:2281:C:OP2	2.40	0.43
5:A:1933:A:O2'	5:A:1934:A:O5'	2.34	0.43
5:A:2302:C:H3'	5:A:2303:G:H5"	2.01	0.43
9:E:133:LEU:O	9:E:137:LEU:HD23	2.18	0.43
10:F:85:ILE:O	10:F:85:ILE:HG13	2.19	0.43
42:l:74:LEU:HD21	42:l:104:CYS:HB2	2.00	0.43
5:A:303:C:H5"	5:A:336:U:H2'	1.99	0.43
31:a:425:U:O2'	31:a:426:A:OP2	2.33	0.43
31:a:754:U:H2'	31:a:755:G:O4'	2.19	0.43
3:2:31:ILE:O	3:2:35:LYS:NZ	2.39	0.43
5:A:91:A:H1'	5:A:92:G:OP2	2.18	0.43
5:A:1575:C:H2'	5:A:1576:U:C1'	2.49	0.43
23:S:14:VAL:HG22	23:S:32:LYS:HG3	2.01	0.43
5:A:1862:A:N6	5:A:1871:G:O2'	2.45	0.43
21:Q:66:HIS:CE1	21:Q:94:THR:HG1	2.36	0.43
31:a:489:C:H2'	31:a:490:A:C8	2.54	0.43
31:a:817:U:H4'	31:a:818:G:OP2	2.19	0.43
34:d:122:HIS:O	34:d:123:ARG:HB2	2.17	0.43
37:g:75:VAL:HG12	37:g:88:PRO:HA	1.99	0.43
5:A:2234:G:H2'	5:A:2234:G:N3	2.34	0.43
10:F:162:THR:HG22	10:F:163:ASP:N	2.34	0.43
19:O:6:PRO:HA	19:O:9:GLN:HG2	2.00	0.43
31:a:140:G:H2'	31:a:141:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:139:ARG:O	32:b:143:MET:HG3	2.19	0.43
36:f:29:ILE:HD11	36:f:74:LEU:HD11	2.00	0.43
5:A:666:A:H2'	5:A:668:A:H62	1.84	0.43
5:A:953:G:N7	16:L:14:LYS:NZ	2.67	0.43
5:A:2795:A:O2'	5:A:2797:G:OP2	2.36	0.43
11:G:86:LYS:HD2	11:G:130:GLU:OE2	2.19	0.43
31:a:1376:G:O2'	31:a:1377:U:H5'	2.19	0.42
5:A:742:C:OP1	8:D:140:SER:O	2.37	0.42
5:A:1341:G:H2'	5:A:1342:A:O4'	2.19	0.42
5:A:2372:A:N3	18:N:110:ARG:NH2	2.67	0.42
36:f:71:LEU:C	36:f:75:GLU:OE1	2.63	0.42
5:A:831:A:H2'	5:A:832:G:C8	2.54	0.42
5:A:2827:G:N2	5:A:2880:U:OP2	2.52	0.42
25:U:4:PHE:HZ	25:U:59:VAL:HG23	1.84	0.42
3:2:28:LYS:HZ2	3:2:40:ILE:HA	1.83	0.42
5:A:368:C:C4'	5:A:369:G:OP2	2.67	0.42
5:A:1044:G:C2'	5:A:1108:A:H61	2.32	0.42
6:B:33:U:O2	6:B:33:U:H2'	2.19	0.42
9:E:153:ASP:OD1	9:E:154:GLU:N	2.52	0.42
43:m:53:LEU:O	43:m:57:ARG:HD2	2.20	0.42
24:T:50:THR:O	24:T:50:THR:HG22	2.20	0.42
31:a:1179:G:C4'	31:a:1180:C:OP2	2.68	0.42
5:A:1172:U:OP2	5:A:1173:G:N2	2.53	0.42
5:A:1519:U:H4'	5:A:1520:A:OP2	2.18	0.42
7:C:146:LEU:HD21	7:C:154:LEU:HD11	2.01	0.42
9:E:1:MET:N	9:E:12:GLU:OE2	2.52	0.42
10:F:38:MET:SD	10:F:53:ALA:HB1	2.60	0.42
10:F:156:ILE:O	10:F:156:ILE:HG13	2.20	0.42
31:a:85:G:C2'	31:a:86:C:OP2	2.66	0.42
31:a:1222:A:H2'	31:a:1223:C:C5	2.55	0.42
5:A:981:A:N3	5:A:981:A:H2'	2.34	0.42
9:E:111:LEU:HD21	9:E:116:ARG:HH21	1.84	0.42
10:F:169:LEU:C	10:F:169:LEU:HD23	2.45	0.42
31:a:1374:A:C5	37:g:7:VAL:HG21	2.55	0.42
32:b:22:THR:O	32:b:25:TRP:N	2.53	0.42
42:l:87:VAL:O	42:l:88:LYS:HB3	2.19	0.42
44:n:33:ASN:OD1	44:n:34:VAL:N	2.53	0.42
31:a:943:A:H2'	31:a:944:G:C8	2.55	0.42
13:I:58:ASN:N	13:I:127:GLY:O	2.48	0.42
31:a:572:G:H4'	31:a:573:C:O5'	2.20	0.42
4:3:3:VAL:HG12	4:3:37:GLN:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1166:A:H2'	5:A:1167:U:C6	2.55	0.42
10:F:57:MET:HA	10:F:60:ILE:HG12	2.02	0.42
12:H:5:LEU:HD23	12:H:36:ALA:HB2	2.01	0.42
31:a:185:C:H1'	31:a:186:G:OP2	2.19	0.42
36:f:85:ILE:O	36:f:86:ARG:CB	2.67	0.42
5:A:19:U:O2	5:A:2622:C:H4'	2.20	0.41
5:A:68:A:C6	5:A:102:A:N1	2.88	0.41
5:A:1193:U:C2	5:A:1194:U:C5	3.08	0.41
5:A:1277:U:H2'	5:A:1278:G:O4'	2.20	0.41
5:A:2237:A:H2'	5:A:2238:G:C8	2.55	0.41
6:B:11:A:N1	6:B:67:G:O2'	2.44	0.41
10:F:9:ASN:HA	10:F:13:LYS:HD3	2.02	0.41
14:J:113:LYS:O	14:J:117:LEU:HD13	2.20	0.41
31:a:567:G:O3'	31:a:816:A:O2'	2.34	0.41
37:g:40:GLU:OE2	39:i:41:THR:HG21	2.21	0.41
44:n:73:TYR:O	44:n:79:LEU:O	2.39	0.41
5:A:903:A:H3'	5:A:904:U:H5"	2.03	0.41
5:A:1044:G:H2'	5:A:1108:A:H61	1.85	0.41
5:A:1296:A:C4'	5:A:1297:A:OP1	2.68	0.41
5:A:2456:U:C2	5:A:2457:A:C8	3.08	0.41
5:A:2699:C:C2	5:A:2700:C:C5	3.08	0.41
11:G:12:PRO:O	11:G:13:ASN:HB3	2.20	0.41
12:H:41:GLU:HG2	12:H:42:ALA:N	2.36	0.41
31:a:670:A:H2'	31:a:671:G:H8	1.85	0.41
32:b:221:ASP:OD1	32:b:221:ASP:C	2.61	0.41
37:g:15:ASP:OD1	37:g:44:TYR:OH	2.39	0.41
5:A:1313:U:C2	5:A:1314:C:C5	3.09	0.41
9:E:116:ARG:O	9:E:116:ARG:HG2	2.21	0.41
31:a:1145:U:H2'	31:a:1146:U:O4'	2.20	0.41
31:a:1433:U:C2	31:a:1434:A:C8	3.08	0.41
37:g:74:GLU:HG3	37:g:75:VAL:N	2.35	0.41
1:0:40:ARG:O	1:0:41:GLN:NE2	2.50	0.41
5:A:314:G:C2	5:A:315:U:C6	3.08	0.41
5:A:2021:C:H2'	5:A:2022:U:C6	2.55	0.41
31:a:459:U:H5"	31:a:460:U:OP1	2.20	0.41
31:a:1123:U:C2'	31:a:1124:G:OP1	2.68	0.41
31:a:1237:U:C5	37:g:116:MET:HE3	2.54	0.41
5:A:235:U:O2	5:A:235:U:O4'	2.38	0.41
5:A:462:G:N2	5:A:465:A:OP2	2.38	0.41
7:C:94:LEU:HD11	7:C:104:ILE:HD13	2.03	0.41
29:Y:46:MET:O	29:Y:50:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Z:3:VAL:HG22	30:Z:4:GLN:N	2.35	0.41
31:a:964:5MC:H5"	31:a:965:A:OP2	2.21	0.41
32:b:71:PHE:CE1	32:b:219:MET:HE2	2.56	0.41
32:b:113:ILE:CD1	32:b:150:LEU:HD12	2.51	0.41
36:f:72:ASP:HA	36:f:75:GLU:OE1	2.21	0.41
40:j:7:ARG:HG3	40:j:73:LEU:HD11	2.02	0.41
5:A:2247:OMG:HM23	5:A:2247:OMG:H1'	1.82	0.41
10:F:31:ILE:O	10:F:31:ILE:CG2	2.68	0.41
10:F:141:ILE:HG22	10:F:142:ASP:H	1.86	0.41
24:T:24:VAL:HG13	24:T:24:VAL:O	2.21	0.41
32:b:49:VAL:CG2	32:b:50:PRO:HD3	2.50	0.41
5:A:537:A:H2'	5:A:538:G:O4'	2.21	0.41
5:A:579:C:H2'	5:A:580:A:H8	1.86	0.41
5:A:1835:G:C2	5:A:1836:G:C8	3.09	0.41
5:A:2529:C:OP1	5:A:2661:A:O2'	2.36	0.41
5:A:2853:G:N2	5:A:2856:A:OP2	2.48	0.41
11:G:71:VAL:HG22	11:G:75:LEU:HD13	2.03	0.41
13:I:105:VAL:HG21	13:I:122:MET:SD	2.61	0.41
31:a:184:A:H3'	31:a:185:C:H5'	2.02	0.41
31:a:457:A:C2	31:a:458:G:C8	3.08	0.41
31:a:577:C:H2'	31:a:578:G:O4'	2.21	0.41
32:b:113:ILE:HD11	32:b:153:VAL:HG13	2.03	0.41
32:b:131:LEU:HD23	32:b:135:GLU:HG2	2.03	0.41
32:b:145:LYS:CE	32:b:146:LEU:HD12	2.50	0.41
33:c:134:MET:HE3	33:c:151:VAL:HG12	2.03	0.41
5:A:33:G:H2'	5:A:34:G:O4'	2.21	0.41
5:A:37:G:O2'	5:A:1209:A:N3	2.48	0.41
5:A:507:U:C4'	5:A:508:C:OP2	2.69	0.41
5:A:1902:G:C8	5:A:1925:G:H2'	2.55	0.41
7:C:71:LYS:HE3	7:C:74:VAL:HG21	2.03	0.41
10:F:121:SER:OG	10:F:121:SER:O	2.39	0.41
10:F:162:THR:HG22	10:F:163:ASP:H	1.86	0.41
17:M:20:MET:HE2	17:M:20:MET:HB3	2.00	0.41
17:M:21:PHE:CZ	17:M:43:GLU:OE1	2.74	0.41
31:a:179:G:C5	31:a:180:U:C6	3.09	0.41
31:a:588:U:H2'	31:a:589:A:C8	2.56	0.41
31:a:915:A:H2'	31:a:916:A:O4'	2.21	0.41
31:a:993:A:H2'	31:a:994:U:C6	2.56	0.41
31:a:1072:U:H2'	31:a:1073:C:C6	2.55	0.41
31:a:1154:A:C2	31:a:1178:G:C4	3.09	0.41
33:c:211:MET:SD	33:c:216:ASN:ND2	2.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:121:ALA:O	37:g:125:LEU:HD23	2.21	0.41
40:j:22:ALA:O	40:j:26:VAL:HG23	2.20	0.41
45:o:40:GLN:O	45:o:44:LYS:NZ	2.54	0.41
45:o:74:ASP:OD1	45:o:74:ASP:C	2.64	0.41
5:A:573:A:C2	5:A:574:U:C5	3.09	0.41
5:A:605:U:C5	5:A:618:G:C5	3.09	0.41
5:A:726:G:H3'	5:A:727:G:C5'	2.51	0.41
5:A:2568:A:C4'	5:A:2569:C:OP2	2.68	0.41
11:G:92:VAL:HG13	11:G:92:VAL:O	2.21	0.41
16:L:133:THR:HG22	16:L:134:ARG:N	2.36	0.41
31:a:1320:G:H2'	31:a:1321:A:C8	2.55	0.41
37:g:70:ARG:HD3	37:g:96:ARG:HB3	2.03	0.41
44:n:72:GLY:O	44:n:80:SER:HA	2.21	0.41
5:A:1793:C:OP1	7:C:273:VAL:HG22	2.22	0.40
7:C:260:ASN:OD1	7:C:262:ARG:N	2.48	0.40
31:a:4:A:H1'	31:a:610:C:O2'	2.21	0.40
31:a:156:A:N6	31:a:342:G:C6	2.89	0.40
31:a:425:U:O2	31:a:426:A:C8	2.75	0.40
31:a:1448:C:O2	31:a:1448:C:O4'	2.39	0.40
32:b:71:PHE:CZ	32:b:219:MET:HE2	2.55	0.40
4:3:27:CYS:CB	4:3:33:HIS:HB2	2.51	0.40
5:A:1776:A:OP1	55:A:3427:HOH:O	2.22	0.40
5:A:2287:U:OP1	5:A:2376:U:O2'	2.39	0.40
5:A:2784:C:O2'	5:A:2805:A:N3	2.48	0.40
6:B:64:A:H5"	6:B:65:G:OP1	2.21	0.40
36:f:71:LEU:O	36:f:74:LEU:N	2.55	0.40
39:i:113:LYS:HB2	39:i:116:LEU:HD12	2.03	0.40
41:k:99:LEU:O	41:k:102:VAL:HG12	2.21	0.40
5:A:1715:G:N1	5:A:1738:U:C2	2.90	0.40
5:A:2762:G:C2	5:A:2763:C:C6	3.10	0.40
31:a:90:C:H2'	31:a:91:G:C8	2.57	0.40
31:a:189:A:O2'	50:t:59:ASP:OD1	2.31	0.40
31:a:725:A:C8	45:o:54:ARG:CZ	3.05	0.40
31:a:980:A:H5'	31:a:981:C:OP2	2.22	0.40
38:h:114:ASP:OD2	38:h:118:ARG:NH1	2.54	0.40
5:A:740:G:H2'	5:A:741:U:C6	2.55	0.40
5:A:1786:U:H2'	5:A:1787:A:C8	2.56	0.40
5:A:1792:U:H2'	5:A:1793:C:C6	2.56	0.40
5:A:2727:G:H2'	5:A:2728:G:C8	2.57	0.40
8:D:86:THR:CG2	8:D:87:GLU:N	2.84	0.40
23:S:17:GLU:O	23:S:21:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:925:G:H2'	31:a:926:G:O4'	2.20	0.40
4:3:36:ARG:O	4:3:37:GLN:HB2	2.21	0.40
5:A:75:G:H2'	5:A:76:C:O4'	2.22	0.40
5:A:961:C:O2'	5:A:2269:A:N3	2.52	0.40
5:A:1493:C:O4'	5:A:1575:C:H4'	2.22	0.40
5:A:2371:G:N2	5:A:2374:A:OP2	2.51	0.40
31:a:83:U:O2'	31:a:84:U:O2	2.24	0.40
47:q:24:VAL:HG11	47:q:62:ILE:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	C	270/274 (98%)	263 (97%)	6 (2%)	1 (0%)	30	39
8	D	209/212 (99%)	200 (96%)	9 (4%)	0	100	100
9	E	198/200 (99%)	197 (100%)	1 (0%)	0	100	100
10	F	172/178 (97%)	152 (88%)	20 (12%)	0	100	100
11	G	172/177 (97%)	163 (95%)	7 (4%)	2 (1%)	10	13
12	H	58/148 (39%)	55 (95%)	3 (5%)	0	100	100
13	I	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	J	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
15	K	142/146 (97%)	137 (96%)	4 (3%)	1 (1%)	18	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	L	135/137 (98%)	132 (98%)	2 (2%)	1 (1%)	18 25
17	M	117/125 (94%)	115 (98%)	2 (2%)	0	100 100
18	N	112/116 (97%)	109 (97%)	3 (3%)	0	100 100
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100 100
20	P	115/119 (97%)	115 (100%)	0	0	100 100
21	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100 100
22	R	107/109 (98%)	105 (98%)	2 (2%)	0	100 100
23	S	89/106 (84%)	87 (98%)	2 (2%)	0	100 100
24	T	101/105 (96%)	99 (98%)	2 (2%)	0	100 100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100 100
26	V	75/85 (88%)	74 (99%)	1 (1%)	0	100 100
27	W	75/78 (96%)	75 (100%)	0	0	100 100
28	X	58/65 (89%)	58 (100%)	0	0	100 100
29	Y	55/58 (95%)	55 (100%)	0	0	100 100
30	Z	53/61 (87%)	51 (96%)	2 (4%)	0	100 100
32	b	223/250 (89%)	210 (94%)	12 (5%)	1 (0%)	30 39
33	c	213/250 (85%)	206 (97%)	7 (3%)	0	100 100
34	d	205/208 (99%)	198 (97%)	6 (3%)	1 (0%)	24 34
35	e	153/165 (93%)	152 (99%)	1 (1%)	0	100 100
36	f	102/127 (80%)	94 (92%)	5 (5%)	3 (3%)	3 3
37	g	139/156 (89%)	138 (99%)	1 (1%)	0	100 100
38	h	128/131 (98%)	124 (97%)	4 (3%)	0	100 100
39	i	124/128 (97%)	121 (98%)	3 (2%)	0	100 100
40	j	98/103 (95%)	94 (96%)	4 (4%)	0	100 100
41	k	115/128 (90%)	111 (96%)	4 (4%)	0	100 100
42	l	120/124 (97%)	110 (92%)	9 (8%)	1 (1%)	16 22
43	m	113/118 (96%)	110 (97%)	3 (3%)	0	100 100
44	n	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
45	o	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
46	p	80/101 (79%)	79 (99%)	1 (1%)	0	100 100
47	q	77/85 (91%)	76 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	r	50/75 (67%)	49 (98%)	1 (2%)	0	100	100
49	s	80/91 (88%)	79 (99%)	1 (1%)	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	61/71 (86%)	60 (98%)	1 (2%)	0	100	100
All	All	5420/5872 (92%)	5256 (97%)	153 (3%)	11 (0%)	44	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	G	81	GLU
32	b	8	MET
36	f	33	ASP
42	l	88	LYS
11	G	13	ASN
36	f	94	HIS
15	K	31	LYS
34	d	128	ASN
36	f	86	ARG
7	C	3	ILE
16	L	78	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	47 (100%)	0	100	100
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	218/220 (99%)	218 (100%)	0	100	100
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	155/155 (100%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	F	144/147 (98%)	144 (100%)	0	100	100
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	118/118 (100%)	118 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	106 (100%)	0	100	100
16	L	113/113 (100%)	113 (100%)	0	100	100
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	98/102 (96%)	98 (100%)	0	100	100
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	77/87 (88%)	77 (100%)	0	100	100
24	T	83/85 (98%)	83 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	60/64 (94%)	60 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	53 (100%)	0	100	100
29	Y	53/54 (98%)	53 (100%)	0	100	100
30	Z	47/50 (94%)	47 (100%)	0	100	100
32	b	185/200 (92%)	184 (100%)	1 (0%)	81	88
33	c	175/198 (88%)	175 (100%)	0	100	100
34	d	170/171 (99%)	170 (100%)	0	100	100
35	e	113/120 (94%)	113 (100%)	0	100	100
36	f	94/111 (85%)	94 (100%)	0	100	100
37	g	118/128 (92%)	118 (100%)	0	100	100
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	99 (100%)	0	100	100
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	l	104/106 (98%)	104 (100%)	0	100	100
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	63 (100%)	0	100	100
47	q	71/76 (93%)	71 (100%)	0	100	100
48	r	46/66 (70%)	46 (100%)	0	100	100
49	s	70/78 (90%)	70 (100%)	0	100	100
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	54/62 (87%)	54 (100%)	0	100	100
All	All	4489/4756 (94%)	4488 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	b	111	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	16	HIS
7	C	134	ASN
7	C	200	ASN
8	D	108	GLN
8	D	143	HIS
9	E	114	GLN
9	E	165	HIS
10	F	63	GLN
11	G	74	ASN
17	M	31	HIS
17	M	57	ASN
19	O	59	ASN
21	Q	69	HIS
22	R	62	ASN
27	W	16	ASN
27	W	35	HIS
32	b	85	GLN

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Mol	Chain	Res	Type
32	b	170	HIS
33	c	18	HIS
33	c	123	GLN
34	d	56	GLN
34	d	148	HIS
36	f	35	GLN
36	f	94	HIS
37	g	21	GLN
44	n	82	ASN
46	p	64	GLN
49	s	56	ASN
50	t	20	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	222 (14%)	0
5	A	2726/2918 (93%)	457 (16%)	30 (1%)
6	B	114/115 (99%)	18 (15%)	2 (1%)
All	All	4367/4577 (95%)	697 (15%)	32 (0%)

All (697) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	U
5	A	20	A
5	A	41	U
5	A	53	G
5	A	56	A
5	A	66	U
5	A	67	G
5	A	68	A
5	A	70	A
5	A	78	A
5	A	81	A
5	A	82	G
5	A	83	C
5	A	92	G
5	A	102	A
5	A	106	U
5	A	107	U

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Mol	Chain	Res	Type
5	A	109	G
5	A	117	G
5	A	125	A
5	A	127	U
5	A	147	A
5	A	149	G
5	A	153	G
5	A	165	U
5	A	170	A
5	A	172	A
5	A	188	A
5	A	203	A
5	A	206	A
5	A	223	A
5	A	228	A
5	A	229	A
5	A	230	A
5	A	235	U
5	A	236	U
5	A	255	G
5	A	257	G
5	A	259	G
5	A	262	A
5	A	272	A
5	A	273	G
5	A	275	C
5	A	278	U
5	A	279	U
5	A	282	G
5	A	303	C
5	A	313	A
5	A	314	G
5	A	324	A
5	A	325	G
5	A	326	A
5	A	331	G
5	A	332	A
5	A	333	U
5	A	335	U
5	A	336	U
5	A	348	A
5	A	359	U

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Mol	Chain	Res	Type
5	A	360	A
5	A	364	A
5	A	365	U
5	A	366	G
5	A	368	C
5	A	369	G
5	A	370	A
5	A	371	G
5	A	372	U
5	A	385	G
5	A	386	U
5	A	395	G
5	A	403	A
5	A	410	G
5	A	416	C
5	A	421	A
5	A	423	G
5	A	435	C
5	A	455	C
5	A	479	A
5	A	480	G
5	A	490	G
5	A	504	A
5	A	507	U
5	A	508	C
5	A	509	C
5	A	526	C
5	A	529	G
5	A	530	C
5	A	531	A
5	A	542	C
5	A	544	U
5	A	545	C
5	A	546	G
5	A	548	G
5	A	554	A
5	A	561	A
5	A	564	U
5	A	571	U
5	A	573	A
5	A	594	A
5	A	595	G

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Mol	Chain	Res	Type
5	A	601	A
5	A	611	U
5	A	612	A
5	A	625	A
5	A	633	C
5	A	635	A
5	A	644	A
5	A	649	G
5	A	651	U
5	A	657	G
5	A	668	A
5	A	684	U
5	A	692	U
5	A	693	G
5	A	703	A
5	A	713	A
5	A	724	G
5	A	728	A
5	A	738	C
5	A	745	U
5	A	746	G
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	787	A
5	A	788	U
5	A	792	G
5	A	800	A
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	826	U
5	A	828	G
5	A	843	G
5	A	851	U
5	A	855	G
5	A	857	G
5	A	874	C
5	A	904	U

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Mol	Chain	Res	Type
5	A	908	A
5	A	912	C
5	A	926	G
5	A	929	C
5	A	930	U
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1002	C
5	A	1006	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1023	G
5	A	1024	A
5	A	1030	U
5	A	1031	G
5	A	1032	U
5	A	1033	G
5	A	1042	U
5	A	1043	A
5	A	1044	G
5	A	1050	U
5	A	1051	A
5	A	1104	G
5	A	1105	U
5	A	1108	A
5	A	1109	G
5	A	1121	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1131	A
5	A	1132	C
5	A	1133	G
5	A	1140	A
5	A	1169	C
5	A	1170	U

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Mol	Chain	Res	Type
5	A	1171	U
5	A	1172	U
5	A	1173	G
5	A	1174	U
5	A	1201	G
5	A	1206	U
5	A	1242	A
5	A	1244	U
5	A	1245	G
5	A	1248	A
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1268	C
5	A	1296	A
5	A	1297	A
5	A	1301	C
5	A	1309	C
5	A	1316	A
5	A	1320	U
5	A	1321	U
5	A	1327	G
5	A	1336	G
5	A	1337	A
5	A	1338	G
5	A	1340	C
5	A	1347	U
5	A	1360	A
5	A	1363	G
5	A	1373	A
5	A	1374	U
5	A	1378	A
5	A	1405	U
5	A	1411	G
5	A	1415	U
5	A	1416	G
5	A	1417	A
5	A	1418	G
5	A	1420	G
5	A	1422	A
5	A	1423	C
5	A	1428	A

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Mol	Chain	Res	Type
5	A	1432	C
5	A	1433	U
5	A	1435	A
5	A	1447	G
5	A	1448	U
5	A	1449	U
5	A	1456	C
5	A	1467	G
5	A	1477	U
5	A	1483	U
5	A	1488	C
5	A	1489	A
5	A	1501	C
5	A	1504	U
5	A	1505	A
5	A	1511	A
5	A	1519	U
5	A	1520	A
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1538	A
5	A	1540	C
5	A	1548	U
5	A	1552	U
5	A	1553	G
5	A	1557	U
5	A	1558	G
5	A	1564	A
5	A	1567	A
5	A	1574	U
5	A	1576	U
5	A	1579	G
5	A	1581	U
5	A	1582	U
5	A	1593	G
5	A	1606	A
5	A	1616	A
5	A	1617	G

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Mol	Chain	Res	Type
5	A	1645	U
5	A	1646	U
5	A	1672	G
5	A	1691	U
5	A	1697	G
5	A	1726	C
5	A	1728	C
5	A	1729	U
5	A	1733	U
5	A	1734	G
5	A	1746	G
5	A	1760	G
5	A	1769	A
5	A	1776	A
5	A	1796	C
5	A	1797	A
5	A	1805	A
5	A	1807	G
5	A	1812	C
5	A	1817	A
5	A	1825	A
5	A	1829	C
5	A	1830	U
5	A	1844	A
5	A	1855	U
5	A	1861	U
5	A	1862	A
5	A	1869	G
5	A	1872	A
5	A	1875	C
5	A	1885	A
5	A	1895	A
5	A	1897	A
5	A	1902	G
5	A	1908	A
5	A	1909	A
5	A	1910	C
5	A	1911	3TD
5	A	1915	A
5	A	1917	G
5	A	1918	G
5	A	1919	U

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Mol	Chain	Res	Type
5	A	1923	A
5	A	1925	G
5	A	1926	G
5	A	1927	U
5	A	1934	A
5	A	1936	U
5	A	1950	G
5	A	1951	U
5	A	1959	U
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1978	U
5	A	1987	U
5	A	1989	U
5	A	2018	U
5	A	2019	C
5	A	2025	G
5	A	2026	6MZ
5	A	2027	A
5	A	2029	A
5	A	2030	U
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2065	G7M
5	A	2089	G
5	A	2194	A
5	A	2200	G
5	A	2204	C
5	A	2207	G
5	A	2210	C
5	A	2221	A
5	A	2234	G
5	A	2236	U
5	A	2261	U
5	A	2279	U
5	A	2283	A

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Mol	Chain	Res	Type
5	A	2284	A
5	A	2299	G
5	A	2301	U
5	A	2303	G
5	A	2305	A
5	A	2307	A
5	A	2308	U
5	A	2314	G
5	A	2316	A
5	A	2317	G
5	A	2321	A
5	A	2323	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2355	C
5	A	2371	G
5	A	2378	G
5	A	2379	G
5	A	2380	U
5	A	2381	C
5	A	2398	U
5	A	2399	C
5	A	2402	U
5	A	2420	C
5	A	2422	A
5	A	2425	G
5	A	2426	A
5	A	2427	U
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2443	G
5	A	2444	A
5	A	2446	A
5	A	2455	A
5	A	2465	A
5	A	2466	G
5	A	2469	U
5	A	2470	U
5	A	2471	C
5	A	2472	A

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Mol	Chain	Res	Type
5	A	2475	U
5	A	2476	C
5	A	2490	G
5	A	2494	C
5	A	2498	G
5	A	2499	2MA
5	A	2501	G
5	A	2502	U
5	A	2503	C
5	A	2514	A
5	A	2516	C
5	A	2525	G
5	A	2543	A
5	A	2548	OMU
5	A	2550	U
5	A	2562	A
5	A	2563	G
5	A	2568	A
5	A	2569	C
5	A	2578	G
5	A	2582	U
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2606	C
5	A	2609	U
5	A	2625	U
5	A	2635	A
5	A	2642	C
5	A	2657	G
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2709	C
5	A	2710	G
5	A	2722	U
5	A	2725	U
5	A	2729	A
5	A	2735	U
5	A	2744	A
5	A	2754	A

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Mol	Chain	Res	Type
5	A	2762	G
5	A	2774	A
5	A	2777	A
5	A	2793	U
5	A	2794	U
5	A	2796	U
5	A	2797	G
5	A	2814	U
5	A	2816	G
5	A	2830	G
5	A	2831	A
5	A	2845	G
5	A	2851	U
5	A	2853	G
5	A	2857	U
5	A	2863	A
5	A	2868	G
5	A	2879	A
5	A	2880	U
5	A	2897	C
6	B	13	A
6	B	14	G
6	B	23	A
6	B	33	U
6	B	39	C
6	B	40	C
6	B	42	G
6	B	43	A
6	B	44	A
6	B	50	A
6	B	51	A
6	B	64	A
6	B	65	G
6	B	71	A
6	B	86	U
6	B	87	A
6	B	88	C
6	B	106	A
31	a	6	C
31	a	11	G
31	a	20	C
31	a	34	A

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Mol	Chain	Res	Type
31	a	41	G
31	a	49	C
31	a	50	U
31	a	52	A
31	a	53	A
31	a	57	A
31	a	62	A
31	a	64	U
31	a	66	G
31	a	80	A
31	a	83	U
31	a	84	U
31	a	85	G
31	a	86	C
31	a	87	U
31	a	90	C
31	a	91	G
31	a	95	C
31	a	97	A
31	a	105	A
31	a	106	C
31	a	107	G
31	a	126	A
31	a	127	U
31	a	140	G
31	a	156	A
31	a	159	G
31	a	160	G
31	a	165	C
31	a	184	A
31	a	185	C
31	a	186	G
31	a	193	A
31	a	200	G
31	a	203	C
31	a	205	U
31	a	208	G
31	a	236	C
31	a	241	U
31	a	243	G
31	a	247	G
31	a	262	G

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Mol	Chain	Res	Type
31	a	263	C
31	a	269	A
31	a	276	C
31	a	285	G
31	a	289	G
31	a	324	C
31	a	337	C
31	a	340	A
31	a	341	C
31	a	343	G
31	a	348	C
31	a	350	G
31	a	359	A
31	a	363	U
31	a	368	C
31	a	369	A
31	a	402	G
31	a	407	A
31	a	408	A
31	a	409	G
31	a	418	A
31	a	419	U
31	a	425	U
31	a	426	A
31	a	447	A
31	a	460	U
31	a	461	A
31	a	463	U
31	a	469	G
31	a	478	G
31	a	481	G
31	a	483	U
31	a	493	A
31	a	494	U
31	a	496	A
31	a	508	C
31	a	509	U
31	a	513	PSU
31	a	515	C
31	a	518	G
31	a	522	C
31	a	524	G7M

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Mol	Chain	Res	Type
31	a	527	G
31	a	528	U
31	a	532	A
31	a	544	A
31	a	561	C
31	a	569	A
31	a	570	A
31	a	573	C
31	a	593	A
31	a	615	C
31	a	630	G
31	a	639	A
31	a	650	A
31	a	662	A
31	a	678	A
31	a	684	A
31	a	685	G
31	a	700	G
31	a	720	U
31	a	721	G
31	a	728	G
31	a	729	C
31	a	731	G
31	a	752	G
31	a	774	A
31	a	778	A
31	a	790	U
31	a	791	A
31	a	810	U
31	a	812	A
31	a	814	C
31	a	816	A
31	a	817	U
31	a	839	U
31	a	841	G
31	a	846	U
31	a	887	G
31	a	888	U
31	a	911	A
31	a	923	G
31	a	924	G
31	a	926	G

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Mol	Chain	Res	Type
31	a	931	C
31	a	932	A
31	a	957	U
31	a	958	U
31	a	963	2MG
31	a	965	A
31	a	966	A
31	a	968	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	989	U
31	a	990	G
31	a	1001	A
31	a	1007	U
31	a	1023	G
31	a	1026	U
31	a	1027	U
31	a	1029	G
31	a	1030	G
31	a	1050	G
31	a	1051	C
31	a	1052	A
31	a	1062	U
31	a	1068	C
31	a	1069	G
31	a	1076	G
31	a	1077	A
31	a	1083	U
31	a	1085	G
31	a	1086	G
31	a	1091	G
31	a	1092	U
31	a	1098	A
31	a	1101	G
31	a	1122	U
31	a	1124	G
31	a	1130	A
31	a	1136	G
31	a	1140	G
31	a	1154	A
31	a	1156	U

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Mol	Chain	Res	Type
31	a	1165	C
31	a	1166	A
31	a	1173	A
31	a	1179	G
31	a	1180	C
31	a	1181	G
31	a	1185	A
31	a	1188	A
31	a	1193	A
31	a	1194	A
31	a	1206	C
31	a	1209	U
31	a	1210	A
31	a	1217	G
31	a	1224	A
31	a	1235	A
31	a	1238	G
31	a	1250	G
31	a	1255	G
31	a	1276	A
31	a	1277	A
31	a	1284	A
31	a	1295	U
31	a	1297	G
31	a	1300	C
31	a	1317	C
31	a	1350	G
31	a	1360	A
31	a	1361	U
31	a	1367	G
31	a	1375	C
31	a	1378	U
31	a	1394	C
31	a	1395	A
31	a	1415	A
31	a	1416	G
31	a	1425	A
31	a	1426	C
31	a	1438	A
31	a	1443	A
31	a	1447	G
31	a	1449	A

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Mol	Chain	Res	Type
31	a	1472	G
31	a	1500	A
31	a	1503	U
31	a	1514	G
31	a	1516	MA6
31	a	1517	C
31	a	1526	G
31	a	1527	G

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	91	A
5	A	256	C
5	A	313	A
5	A	324	A
5	A	334	A
5	A	365	U
5	A	368	C
5	A	370	A
5	A	371	G
5	A	424	G
5	A	478	A
5	A	507	U
5	A	782	G
5	A	799	G
5	A	957	A
5	A	1127	U
5	A	1172	U
5	A	1179	G
5	A	1187	G
5	A	1205	A
5	A	1267	A
5	A	1296	A
5	A	1337	A
5	A	1519	U
5	A	1616	A
5	A	1816	U
5	A	2029	A
5	A	2379	G
5	A	2419	U
5	A	2568	A

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Mol	Chain	Res	Type
6	B	13	A
6	B	86	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

24 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PSU	A	2453	5	18,21,22	1.16	1 (5%)	21,30,33	1.98	6 (28%)
5	PSU	A	952	5	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
31	G7M	a	524	31	23,26,27	1.88	2 (8%)	34,39,42	1.05	1 (2%)
31	MA6	a	1516	31	23,26,27	1.37	4 (17%)	33,38,41	3.24	12 (36%)
5	2MG	A	2441	5	23,26,27	0.45	0	33,38,41	0.49	0
31	2MG	a	963	54,31	23,26,27	0.45	0	33,38,41	0.52	0
5	G7M	A	2065	5	23,26,27	1.89	2 (8%)	34,39,42	1.08	1 (2%)
5	OMU	A	2548	5	19,22,23	3.13	8 (42%)	25,31,34	1.79	5 (20%)
31	2MG	a	1204	31	23,26,27	0.47	0	33,38,41	0.51	0
31	5MC	a	964	31	19,22,23	0.52	0	26,32,35	0.57	0
5	5MU	A	1935	5	19,22,23	0.39	0	27,32,35	0.48	0
5	PSU	A	2576	5	18,21,22	1.14	1 (5%)	21,30,33	1.95	6 (28%)
5	OMG	A	2247	5	23,26,27	0.44	0	32,38,41	0.51	0
31	UR3	a	1495	31	19,22,23	2.97	6 (31%)	26,32,35	1.64	4 (15%)
5	PSU	A	1913	5	18,21,22	1.16	1 (5%)	21,30,33	1.90	5 (23%)
31	MA6	a	1515	31	23,26,27	1.38	4 (17%)	33,38,41	3.21	12 (36%)
31	4OC	a	1399	31	20,23,24	3.21	8 (40%)	25,32,35	0.88	1 (4%)
5	2MA	A	2499	5,54	22,25,26	3.99	9 (40%)	32,37,40	2.75	11 (34%)
5	PSU	A	2601	5	18,21,22	1.14	1 (5%)	21,30,33	1.94	5 (23%)
31	PSU	a	513	31	18,21,22	1.14	1 (5%)	21,30,33	1.94	6 (28%)
5	PSU	A	1907	5	18,21,22	1.14	1 (5%)	21,30,33	1.95	5 (23%)
5	3TD	A	1911	5	19,22,23	4.47	6 (31%)	23,32,35	1.79	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PSU	A	2500	5	18,21,22	1.12	1 (5%)	21,30,33	1.97	5 (23%)
5	6MZ	A	2026	5	22,25,26	2.48	4 (18%)	29,36,39	3.32	10 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
31	G7M	a	524	31	-	2/7/25/26	0/3/3/3
31	MA6	a	1516	31	-	2/11/29/30	0/3/3/3
5	2MG	A	2441	5	-	0/9/27/28	0/3/3/3
31	2MG	a	963	54,31	-	2/9/27/28	0/3/3/3
5	G7M	A	2065	5	-	1/7/25/26	0/3/3/3
5	OMU	A	2548	5	-	1/9/27/28	0/2/2/2
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
5	OMG	A	2247	5	-	0/9/27/28	0/3/3/3
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
5	PSU	A	1913	5	-	2/7/25/26	0/2/2/2
31	MA6	a	1515	31	-	0/11/29/30	0/3/3/3
31	4OC	a	1399	31	-	2/9/29/30	0/2/2/2
5	2MA	A	2499	5,54	-	6/7/25/26	0/3/3/3
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	2/7/25/26	0/2/2/2
5	PSU	A	1907	5	-	2/7/25/26	0/2/2/2
5	3TD	A	1911	5	-	2/7/25/26	0/2/2/2
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
5	6MZ	A	2026	5	-	0/9/27/28	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	13.46	1.50	1.35
5	A	2499	2MA	C4-N3	12.17	1.50	1.34
5	A	1911	3TD	C2-N1	10.77	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2026	6MZ	C6-N6	10.22	1.45	1.34
5	A	2065	G7M	C8-N7	7.54	1.45	1.33
5	A	2499	2MA	C2-N3	7.51	1.46	1.34
31	a	524	G7M	C8-N7	7.51	1.45	1.33
5	A	2548	OMU	C2-N1	7.46	1.50	1.38
31	a	1495	UR3	C2-N1	7.41	1.48	1.38
31	a	1399	4OC	C4-N3	7.19	1.44	1.32
5	A	2499	2MA	C6-N1	7.16	1.44	1.35
5	A	2548	OMU	C2-N3	6.91	1.50	1.38
31	a	1495	UR3	C6-C5	6.77	1.50	1.35
31	a	1399	4OC	C2-N3	6.32	1.48	1.36
31	a	1399	4OC	C6-C5	6.31	1.49	1.35
5	A	2499	2MA	C2-N1	6.16	1.44	1.34
5	A	1911	3TD	C6-N1	5.82	1.45	1.36
31	a	1495	UR3	C2-N3	5.73	1.50	1.39
5	A	2548	OMU	C6-C5	5.71	1.48	1.35
5	A	1911	3TD	C2-N3	4.96	1.49	1.38
31	a	1399	4OC	C4-N4	4.83	1.46	1.36
5	A	2499	2MA	C5-C6	4.76	1.54	1.41
5	A	2548	OMU	C4-N3	4.44	1.46	1.38
31	a	1399	4OC	C2-N1	4.33	1.49	1.40
5	A	2065	G7M	C8-N9	4.09	1.46	1.35
31	a	524	G7M	C8-N9	4.05	1.46	1.35
31	a	1515	MA6	C6-N6	3.98	1.47	1.36
31	a	1516	MA6	C6-N6	3.93	1.47	1.36
5	A	1913	PSU	C6-C5	3.90	1.39	1.35
5	A	2453	PSU	C6-C5	3.82	1.39	1.35
5	A	1907	PSU	C6-C5	3.80	1.39	1.35
31	a	513	PSU	C6-C5	3.77	1.39	1.35
5	A	2576	PSU	C6-C5	3.76	1.39	1.35
5	A	2601	PSU	C6-C5	3.73	1.39	1.35
5	A	2500	PSU	C6-C5	3.71	1.39	1.35
5	A	952	PSU	C6-C5	3.64	1.39	1.35
31	a	1399	4OC	C5-C4	3.61	1.49	1.41
31	a	1495	UR3	C6-N1	3.44	1.46	1.38
31	a	1399	4OC	C6-N1	3.32	1.46	1.38
5	A	2499	2MA	C6-N6	-3.31	1.25	1.34
5	A	1911	3TD	C4-N3	3.10	1.46	1.40
5	A	2026	6MZ	C5-N7	-2.97	1.33	1.39
5	A	2548	OMU	O4-C4	-2.95	1.18	1.24
5	A	2548	OMU	C6-N1	2.94	1.45	1.38
31	a	1515	MA6	C5-C4	-2.79	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1516	MA6	C5-C4	-2.79	1.34	1.39
31	a	1495	UR3	C4-N3	2.75	1.46	1.40
31	a	1399	4OC	O2-C2	-2.64	1.18	1.23
5	A	2026	6MZ	C5-C4	-2.60	1.34	1.39
5	A	2499	2MA	C5-N7	-2.49	1.34	1.39
5	A	2548	OMU	C5-C4	2.45	1.49	1.43
31	a	1515	MA6	C5-N7	-2.37	1.34	1.39
31	a	1516	MA6	C5-N7	-2.35	1.34	1.39
5	A	2548	OMU	O2-C2	-2.35	1.18	1.23
31	a	1495	UR3	C5-C4	2.30	1.49	1.43
5	A	2026	6MZ	C8-N9	-2.22	1.33	1.37
5	A	1911	3TD	O2-C2	-2.20	1.19	1.23
31	a	1515	MA6	C8-N9	-2.15	1.33	1.37
5	A	2499	2MA	C4-N9	-2.15	1.33	1.37
5	A	2499	2MA	C8-N7	2.14	1.35	1.31
31	a	1516	MA6	C8-N9	-2.14	1.33	1.37

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	N1-C6-N6	-11.72	102.58	116.86
31	a	1515	MA6	N1-C6-N6	-11.56	102.77	116.86
5	A	2026	6MZ	C1'-N9-C8	8.52	146.00	127.09
5	A	2026	6MZ	C4-N9-C1'	-8.52	106.72	126.63
31	a	1516	MA6	C5-C6-N6	7.85	137.76	125.33
31	a	1515	MA6	C5-C6-N6	7.81	137.69	125.33
5	A	2499	2MA	C1'-N9-C8	-7.58	110.27	127.09
5	A	2026	6MZ	C5-C4-N3	-6.47	117.81	126.72
5	A	2499	2MA	C5-C4-N3	-5.85	121.02	127.18
31	a	1516	MA6	N1-C2-N3	-5.65	120.03	128.58
31	a	1495	UR3	C4-N3-C2	-5.63	120.05	124.58
5	A	1911	3TD	N1-C2-N3	5.63	120.22	116.13
5	A	2499	2MA	N9-C8-N7	-5.58	106.02	113.94
5	A	2026	6MZ	N1-C2-N3	-5.52	120.23	128.58
31	a	1515	MA6	N1-C2-N3	-5.50	120.26	128.58
5	A	2548	OMU	C4-N3-C2	-5.47	119.82	126.61
5	A	2499	2MA	C4-N9-C1'	5.29	139.01	126.63
5	A	2500	PSU	C4-N3-C2	-4.97	119.53	126.37
5	A	2601	PSU	C4-N3-C2	-4.92	119.59	126.37
5	A	2453	PSU	N1-C2-N3	4.89	120.33	115.17
5	A	1907	PSU	N1-C2-N3	4.88	120.31	115.17
31	a	513	PSU	C4-N3-C2	-4.86	119.67	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	C5-C4-N3	-4.85	120.04	126.72
5	A	2453	PSU	C4-N3-C2	-4.84	119.70	126.37
5	A	2601	PSU	N1-C2-N3	4.84	120.27	115.17
5	A	952	PSU	C4-N3-C2	-4.83	119.72	126.37
5	A	2500	PSU	N1-C2-N3	4.79	120.22	115.17
5	A	1907	PSU	C4-N3-C2	-4.78	119.79	126.37
5	A	952	PSU	N1-C2-N3	4.77	120.20	115.17
5	A	2576	PSU	C4-N3-C2	-4.76	119.81	126.37
5	A	2576	PSU	N1-C2-N3	4.76	120.19	115.17
31	a	513	PSU	N1-C2-N3	4.76	120.19	115.17
31	a	1515	MA6	C5-C4-N3	-4.75	120.17	126.72
5	A	2499	2MA	C4-N9-C8	4.74	110.71	105.74
5	A	1913	PSU	N1-C2-N3	4.74	120.16	115.17
5	A	2026	6MZ	C4-C5-C6	4.73	120.71	116.78
5	A	1913	PSU	C4-N3-C2	-4.69	119.92	126.37
5	A	2026	6MZ	N3-C4-N9	4.42	134.69	127.17
5	A	2499	2MA	N3-C4-N9	4.36	132.52	126.99
5	A	1911	3TD	C4-N3-C2	-4.34	120.02	124.61
5	A	2065	G7M	N9-C8-N7	-4.32	102.00	112.48
31	a	1515	MA6	N9-C8-N7	-4.28	107.87	113.94
31	a	524	G7M	N9-C8-N7	-4.25	102.16	112.48
31	a	1516	MA6	N9-C8-N7	-4.15	108.05	113.94
31	a	1515	MA6	C4-C5-C6	4.01	120.05	115.91
31	a	1516	MA6	C4-C5-C6	3.95	119.99	115.91
5	A	2026	6MZ	C2-N3-C4	3.91	121.39	111.83
5	A	2548	OMU	N3-C2-N1	3.82	119.87	114.89
31	a	1495	UR3	C5-C4-N3	3.69	119.90	115.04
5	A	2026	6MZ	N9-C8-N7	-3.57	108.86	113.94
5	A	2548	OMU	C5-C4-N3	3.51	119.72	114.80
31	a	1515	MA6	C2-N1-C6	3.47	120.30	111.83
31	a	1516	MA6	C2-N1-C6	3.46	120.28	111.83
31	a	1516	MA6	C2-N3-C4	3.35	120.01	111.83
5	A	2499	2MA	C5-N7-C8	3.32	108.67	103.45
5	A	2499	2MA	N3-C2-N1	-3.30	119.94	125.77
31	a	1515	MA6	C2-N3-C4	3.22	119.69	111.83
31	a	1516	MA6	N3-C4-N9	3.00	132.26	127.17
31	a	1515	MA6	N3-C4-N9	2.98	132.23	127.17
5	A	2500	PSU	O2-C2-N1	-2.97	119.73	122.79
5	A	1907	PSU	O2-C2-N1	-2.96	119.74	122.79
5	A	2026	6MZ	C5-N7-C8	2.92	108.04	103.45
31	a	513	PSU	O2-C2-N1	-2.90	119.80	122.79
5	A	2453	PSU	O2-C2-N1	-2.90	119.80	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1515	MA6	C5-N7-C8	2.89	107.99	103.45
5	A	2548	OMU	O4-C4-C5	-2.87	120.21	125.16
31	a	1516	MA6	C5-N7-C8	2.86	107.95	103.45
5	A	2576	PSU	O2-C2-N1	-2.84	119.86	122.79
5	A	1913	PSU	O2-C2-N1	-2.81	119.89	122.79
5	A	2601	PSU	O2-C2-N1	-2.79	119.92	122.79
5	A	952	PSU	O2-C2-N1	-2.68	120.02	122.79
5	A	1907	PSU	C6-N1-C2	-2.55	120.33	122.69
31	a	1515	MA6	C4-N9-C8	2.54	108.41	105.74
5	A	2500	PSU	C6-C5-C4	2.51	119.87	118.17
5	A	1913	PSU	C6-N1-C2	-2.50	120.37	122.69
5	A	2453	PSU	C6-N1-C2	-2.50	120.37	122.69
31	a	1495	UR3	C6-N1-C2	-2.45	119.80	121.80
5	A	2576	PSU	O4'-C1'-C2'	2.44	108.53	105.15
5	A	2026	6MZ	C5-C6-N1	2.38	120.70	118.15
31	a	1399	4OC	C6-C5-C4	2.36	119.85	117.00
5	A	2601	PSU	C6-N1-C2	-2.36	120.50	122.69
5	A	2453	PSU	C6-C5-C4	2.36	119.77	118.17
5	A	2576	PSU	C6-N1-C2	-2.36	120.50	122.69
5	A	952	PSU	C6-N1-C2	-2.34	120.52	122.69
31	a	1516	MA6	C4-N9-C8	2.34	108.19	105.74
5	A	2499	2MA	CM2-C2-N1	2.28	120.54	117.13
5	A	1907	PSU	C6-C5-C4	2.26	119.70	118.17
5	A	2499	2MA	N6-C6-N1	2.25	120.07	117.03
5	A	1911	3TD	C6-C5-C4	2.23	119.69	118.19
5	A	952	PSU	C6-C5-C4	2.23	119.68	118.17
5	A	2453	PSU	O4'-C1'-C2'	2.20	108.19	105.15
31	a	513	PSU	O4'-C1'-C2'	2.19	108.19	105.15
31	a	513	PSU	C6-N1-C2	-2.18	120.66	122.69
5	A	1913	PSU	O4'-C1'-C2'	2.17	108.15	105.15
31	a	1516	MA6	C4-C5-N7	-2.16	108.11	110.58
5	A	2499	2MA	C4-C5-N7	-2.14	108.14	110.58
31	a	1515	MA6	C4-C5-N7	-2.14	108.14	110.58
5	A	2601	PSU	C6-C5-C4	2.08	119.58	118.17
5	A	2576	PSU	C6-C5-C4	2.08	119.58	118.17
31	a	513	PSU	C6-C5-C4	2.06	119.56	118.17
5	A	2500	PSU	C6-N1-C2	-2.06	120.78	122.69
31	a	1495	UR3	C1'-N1-C2	2.02	120.35	117.04
5	A	2548	OMU	O2-C2-N1	-2.00	120.19	122.80

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	513	PSU	O4'-C4'-C5'-O5'
31	a	963	2MG	O4'-C4'-C5'-O5'
5	A	1911	3TD	C3'-C4'-C5'-O5'
5	A	1911	3TD	O4'-C4'-C5'-O5'
31	a	513	PSU	C3'-C4'-C5'-O5'
31	a	524	G7M	C3'-C4'-C5'-O5'
5	A	1913	PSU	C3'-C4'-C5'-O5'
5	A	1913	PSU	O4'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
31	a	524	G7M	O4'-C4'-C5'-O5'
31	a	963	2MG	C3'-C4'-C5'-O5'
31	a	1399	4OC	O4'-C4'-C5'-O5'
31	a	1516	MA6	C3'-C4'-C5'-O5'
5	A	1907	PSU	C3'-C4'-C5'-O5'
5	A	2499	2MA	C4'-C5'-O5'-P
5	A	2548	OMU	C4'-C5'-O5'-P
5	A	2499	2MA	O4'-C1'-N9-C8
5	A	2499	2MA	C2'-C1'-N9-C8
31	a	1399	4OC	C3'-C4'-C5'-O5'
5	A	2499	2MA	C2'-C1'-N9-C4
31	a	1516	MA6	C4'-C5'-O5'-P
5	A	1907	PSU	O4'-C4'-C5'-O5'
5	A	2065	G7M	C4'-C5'-O5'-P

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2548	OMU	1	0
31	a	964	5MC	2	0
5	A	1935	5MU	1	0
5	A	2247	OMG	1	0
5	A	1911	3TD	1	0
5	A	2026	6MZ	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 195 ligands modelled in this entry, 192 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	YQM	A	3201	54	43,44,44	3.68	23 (53%)	53,69,69	2.81	23 (43%)
53	YQM	A	3202	54	43,44,44	3.73	21 (48%)	53,69,69	2.79	23 (43%)
53	YQM	a	1601	54	43,44,44	3.60	21 (48%)	53,69,69	2.76	22 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	YQM	A	3201	54	-	0/16/81/81	0/5/5/5
53	YQM	A	3202	54	-	5/16/81/81	0/5/5/5
53	YQM	a	1601	54	-	4/16/81/81	0/5/5/5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3201	YQM	C19-C20	14.24	1.64	1.52
53	A	3202	YQM	C19-C20	14.18	1.64	1.52
53	a	1601	YQM	C19-C20	14.07	1.64	1.52
53	A	3202	YQM	C19-C17	8.53	1.66	1.55
53	a	1601	YQM	C19-C17	8.35	1.66	1.55
53	a	1601	YQM	C05-C04	8.16	1.62	1.54
53	A	3201	YQM	C05-C04	7.90	1.62	1.54
53	A	3202	YQM	C05-C04	7.79	1.61	1.54
53	A	3201	YQM	C19-C17	7.58	1.65	1.55
53	A	3201	YQM	C21-C24	5.81	1.59	1.47
53	A	3202	YQM	C21-C24	5.74	1.59	1.47
53	a	1601	YQM	C21-C24	5.23	1.58	1.47
53	A	3201	YQM	C19-C05	4.67	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3202	YQM	C19-C05	4.60	1.57	1.53
53	A	3202	YQM	C32-N31	4.58	1.45	1.35
53	A	3201	YQM	C32-N31	4.53	1.45	1.35
53	A	3202	YQM	C09-C10	4.46	1.45	1.38
53	A	3201	YQM	C09-C10	4.46	1.45	1.38
53	a	1601	YQM	C09-C10	4.28	1.44	1.38
53	A	3202	YQM	C14-C15	4.28	1.58	1.45
53	a	1601	YQM	C32-N31	4.24	1.44	1.35
53	A	3201	YQM	C14-C15	4.08	1.57	1.45
53	A	3202	YQM	C17-C16	3.99	1.54	1.46
53	A	3202	YQM	C12-N31	3.94	1.49	1.41
53	A	3202	YQM	C14-C13	3.93	1.49	1.41
53	A	3201	YQM	C14-C13	3.92	1.49	1.41
53	a	1601	YQM	C14-C15	3.86	1.57	1.45
53	A	3201	YQM	C12-N31	3.80	1.49	1.41
53	A	3202	YQM	C15-C16	3.66	1.42	1.36
53	a	1601	YQM	C17-C16	3.60	1.53	1.46
53	a	1601	YQM	C12-N31	3.53	1.48	1.41
53	a	1601	YQM	C14-C13	3.47	1.48	1.41
53	A	3201	YQM	C15-C16	3.47	1.42	1.36
53	a	1601	YQM	C19-C05	3.46	1.56	1.53
53	A	3201	YQM	C17-C16	3.31	1.52	1.46
53	a	1601	YQM	C24-N26	3.19	1.42	1.33
53	A	3201	YQM	C24-N26	3.16	1.42	1.33
53	a	1601	YQM	C15-C16	3.14	1.41	1.36
53	A	3202	YQM	C34-C32	3.14	1.58	1.52
53	A	3202	YQM	C24-N26	3.14	1.42	1.33
53	A	3201	YQM	C21-C22	3.07	1.53	1.44
53	A	3202	YQM	C21-C22	3.01	1.53	1.44
53	A	3201	YQM	C34-C32	3.00	1.57	1.52
53	A	3202	YQM	C12-C13	2.95	1.44	1.40
53	A	3201	YQM	C12-C13	2.94	1.44	1.40
53	a	1601	YQM	C21-C22	2.87	1.53	1.44
53	a	1601	YQM	C12-C13	2.71	1.44	1.40
53	a	1601	YQM	C08-C09	2.71	1.55	1.51
53	a	1601	YQM	C34-C32	2.68	1.57	1.52
53	a	1601	YQM	C04-N02	2.68	1.53	1.47
53	A	3201	YQM	C08-C09	2.66	1.55	1.51
53	A	3201	YQM	C04-N02	2.62	1.52	1.47
53	a	1601	YQM	C36-N35	2.57	1.52	1.47
53	A	3202	YQM	C36-N35	2.54	1.52	1.47
53	A	3202	YQM	C08-C07	2.50	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3202	YQM	C11-C10	2.49	1.41	1.37
53	a	1601	YQM	C11-C10	2.48	1.41	1.37
53	A	3201	YQM	C08-C07	2.47	1.59	1.52
53	A	3202	YQM	C08-C09	2.46	1.55	1.51
53	A	3201	YQM	C11-C10	2.42	1.41	1.37
53	A	3202	YQM	C04-N02	2.42	1.52	1.47
53	A	3201	YQM	C06-C07	2.37	1.58	1.53
53	a	1601	YQM	C08-C07	2.33	1.58	1.52
53	A	3201	YQM	C36-N35	2.28	1.52	1.47
53	A	3201	YQM	C07-C16	2.20	1.53	1.51

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	3201	YQM	C34-N35-C39	-7.64	103.44	113.34
53	A	3202	YQM	C34-C32-N31	7.45	128.01	114.23
53	a	1601	YQM	C34-C32-N31	6.92	127.05	114.23
53	a	1601	YQM	C34-N35-C39	-6.69	104.67	113.34
53	A	3201	YQM	C34-C32-N31	6.68	126.60	114.23
53	A	3202	YQM	C34-N35-C39	-6.64	104.73	113.34
53	A	3201	YQM	C11-C12-C13	-5.84	114.87	120.53
53	A	3202	YQM	C11-C12-C13	-5.84	114.88	120.53
53	a	1601	YQM	C11-C12-C13	-5.81	114.90	120.53
53	a	1601	YQM	O27-C20-C21	5.51	127.49	121.90
53	A	3201	YQM	O18-C17-C16	5.28	129.02	121.47
53	A	3201	YQM	O27-C20-C21	5.16	127.14	121.90
53	A	3202	YQM	O27-C20-C21	5.06	127.04	121.90
53	a	1601	YQM	O18-C17-C19	-4.83	109.92	119.11
53	A	3202	YQM	O33-C32-C34	-4.78	112.65	121.02
53	A	3201	YQM	C07-C06-C05	4.78	118.52	110.38
53	A	3202	YQM	O18-C17-C19	-4.74	110.09	119.11
53	a	1601	YQM	O33-C32-C34	-4.68	112.83	121.02
53	A	3202	YQM	O18-C17-C16	4.64	128.11	121.47
53	a	1601	YQM	C07-C16-C15	-4.48	114.91	121.44
53	a	1601	YQM	C39-N35-C36	4.44	109.28	104.04
53	A	3201	YQM	O33-C32-C34	-4.41	113.31	121.02
53	A	3201	YQM	O18-C17-C19	-4.21	111.11	119.11
53	A	3201	YQM	C21-C24-N26	4.14	127.08	118.64
53	A	3202	YQM	C21-C24-N26	4.12	127.04	118.64
53	a	1601	YQM	C07-C06-C05	4.04	117.27	110.38
53	a	1601	YQM	C21-C24-N26	3.95	126.70	118.64
53	a	1601	YQM	O18-C17-C16	3.92	127.09	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	3202	YQM	C07-C06-C05	3.90	117.02	110.38
53	A	3202	YQM	C07-C16-C15	-3.80	115.90	121.44
53	A	3202	YQM	C19-C20-C21	-3.67	117.62	122.89
53	A	3201	YQM	O25-C24-N26	-3.66	114.69	122.89
53	A	3202	YQM	O25-C24-N26	-3.61	114.80	122.89
53	a	1601	YQM	O25-C24-N26	-3.49	115.06	122.89
53	A	3201	YQM	C39-N35-C36	3.46	108.13	104.04
53	a	1601	YQM	C19-C05-C04	3.42	116.32	111.64
53	A	3202	YQM	C17-C19-C20	3.41	113.88	109.88
53	A	3202	YQM	O27-C20-C19	-3.31	108.58	113.37
53	A	3201	YQM	O27-C20-C19	-3.26	108.65	113.37
53	A	3201	YQM	C06-C05-C04	-3.24	109.05	113.73
53	a	1601	YQM	C14-C13-C12	3.20	124.52	118.98
53	a	1601	YQM	C06-C07-C16	3.20	117.23	110.28
53	A	3202	YQM	C14-C13-C12	3.18	124.48	118.98
53	a	1601	YQM	C06-C05-C04	-3.17	109.15	113.73
53	A	3201	YQM	C14-C13-C12	3.17	124.47	118.98
53	A	3201	YQM	C17-C19-C20	3.11	113.53	109.88
53	A	3201	YQM	C19-C05-C04	3.09	115.87	111.64
53	A	3201	YQM	C24-C21-C22	-3.07	117.21	120.87
53	A	3202	YQM	C19-C05-C04	3.01	115.76	111.64
53	a	1601	YQM	C24-C21-C22	-2.98	117.32	120.87
53	A	3201	YQM	C19-C20-C21	-2.91	118.71	122.89
53	A	3202	YQM	C24-C21-C22	-2.91	117.40	120.87
53	A	3202	YQM	C39-N35-C36	2.90	107.47	104.04
53	A	3202	YQM	C06-C05-C04	-2.80	109.69	113.73
53	A	3201	YQM	C07-C16-C15	-2.66	117.56	121.44
53	a	1601	YQM	C17-C19-C20	2.62	112.95	109.88
53	A	3202	YQM	C06-C07-C16	2.52	115.74	110.28
53	a	1601	YQM	O27-C20-C19	-2.46	109.81	113.37
53	A	3202	YQM	O28-C19-C20	-2.45	106.22	110.14
53	A	3201	YQM	C34-N35-C36	-2.42	110.21	113.34
53	A	3202	YQM	O33-C32-N31	-2.40	119.33	123.64
53	A	3201	YQM	C06-C07-C16	2.32	115.33	110.28
53	a	1601	YQM	C19-C20-C21	-2.26	119.66	122.89
53	A	3201	YQM	O29-C15-C14	-2.16	113.68	118.45
53	A	3202	YQM	O29-C15-C14	-2.13	113.74	118.45
53	a	1601	YQM	O28-C19-C20	-2.11	106.77	110.14
53	A	3201	YQM	O28-C19-C20	-2.09	106.80	110.14
53	a	1601	YQM	O29-C15-C14	-2.08	113.86	118.45

There are no chirality outliers.

All (9) torsion outliers are listed below:

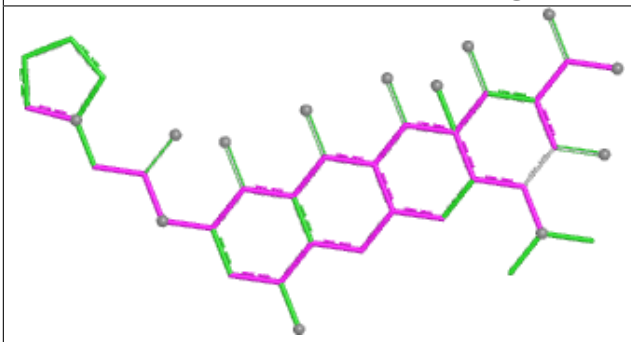
Mol	Chain	Res	Type	Atoms
53	A	3202	YQM	C22-C21-C24-N26
53	a	1601	YQM	C20-C21-C24-N26
53	a	1601	YQM	C20-C21-C24-O25
53	a	1601	YQM	C22-C21-C24-N26
53	a	1601	YQM	C22-C21-C24-O25
53	A	3202	YQM	O33-C32-C34-N35
53	A	3202	YQM	C13-C12-N31-C32
53	A	3202	YQM	N31-C32-C34-N35
53	A	3202	YQM	C22-C21-C24-O25

There are no ring outliers.

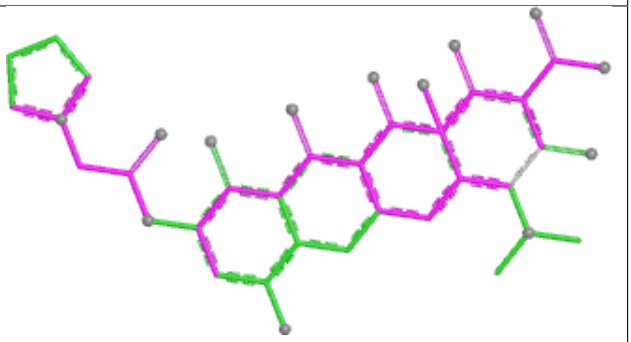
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

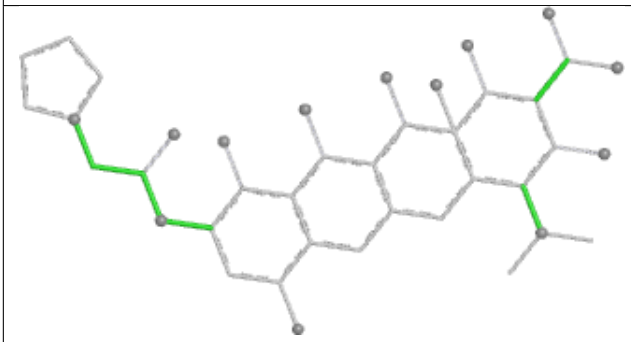
Ligand YQM A 3201



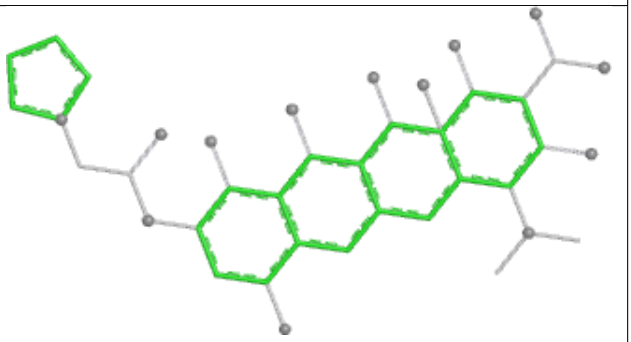
Bond lengths



Bond angles

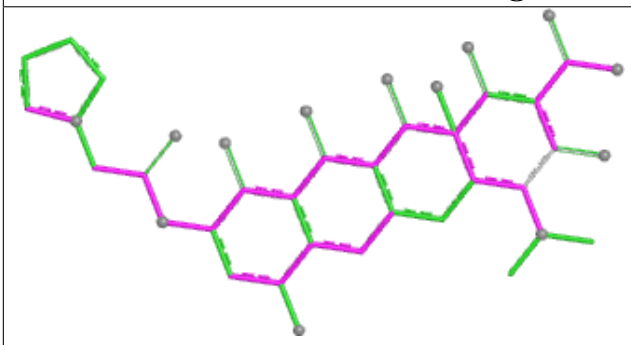


Torsions

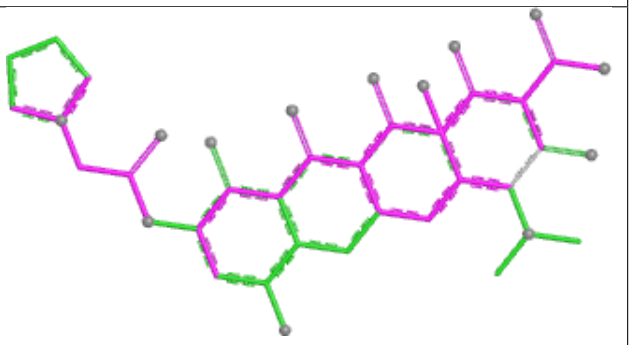


Rings

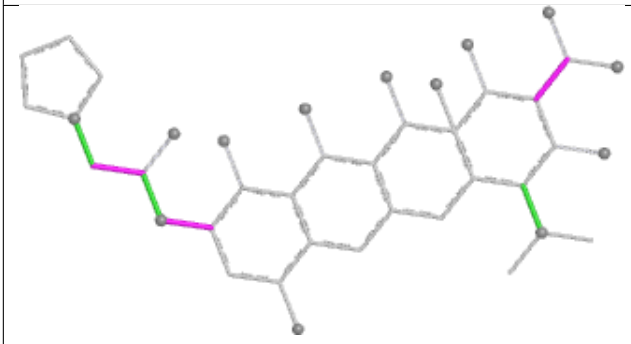
Ligand YQM A 3202



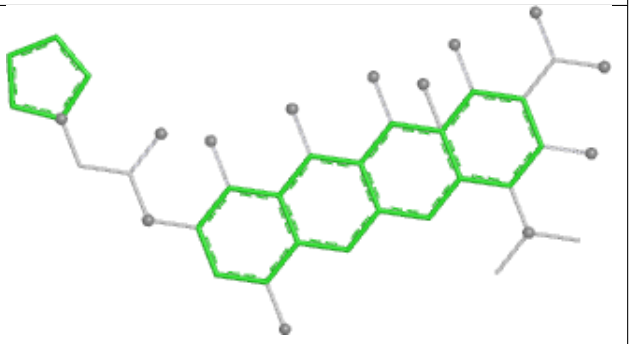
Bond lengths



Bond angles

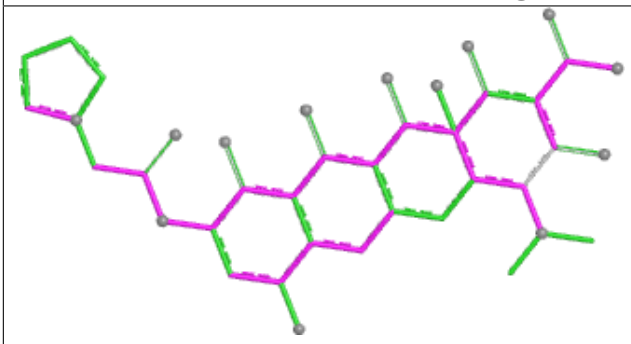


Torsions

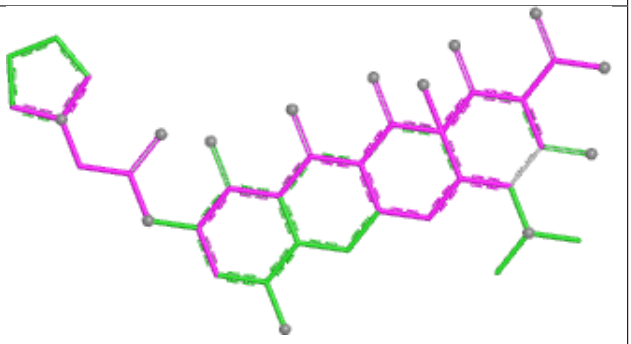


Rings

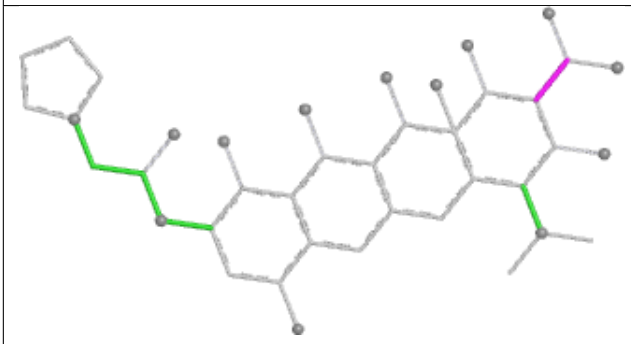
Ligand YQM a 1601



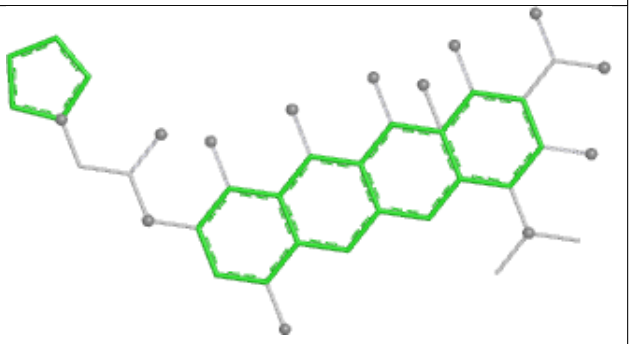
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

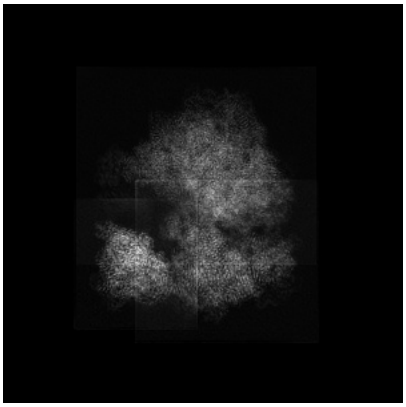
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23668. These allow visual inspection of the internal detail of the map and identification of artifacts.

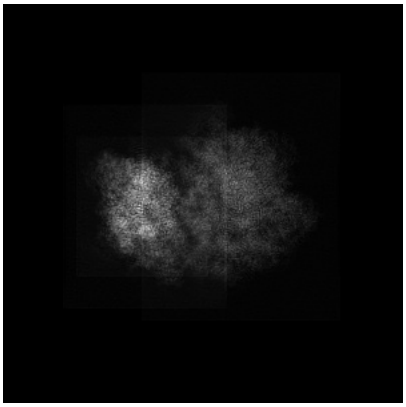
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

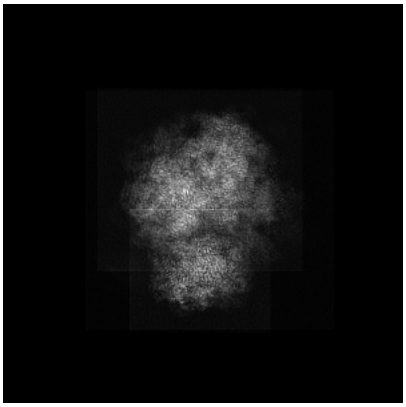
6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices

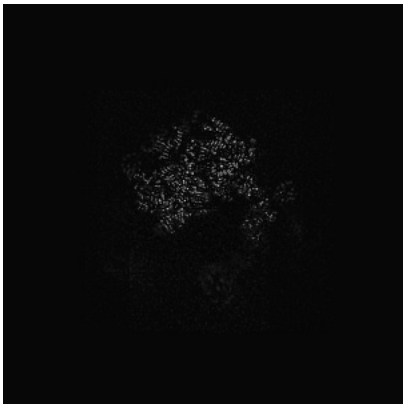
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

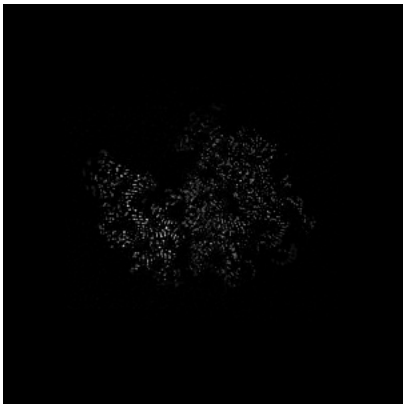
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

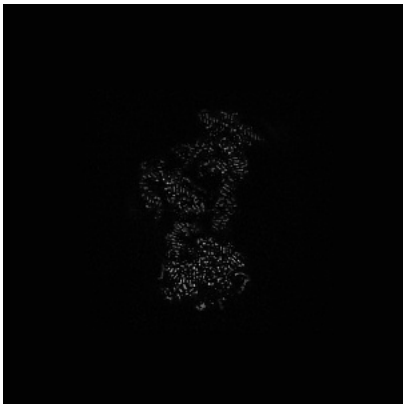
6.3.1 Primary map



X Index: 231



Y Index: 271

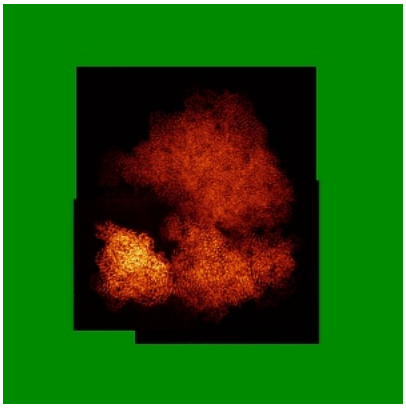


Z Index: 178

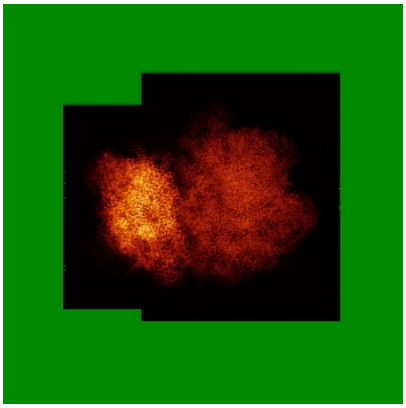
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

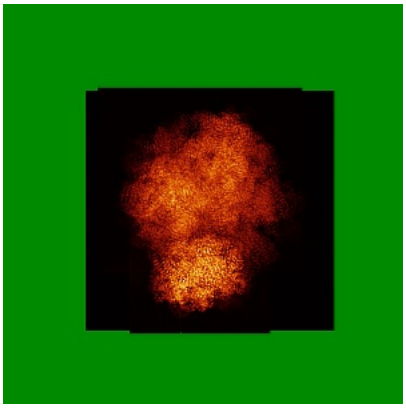
6.4.1 Primary map



X



Y

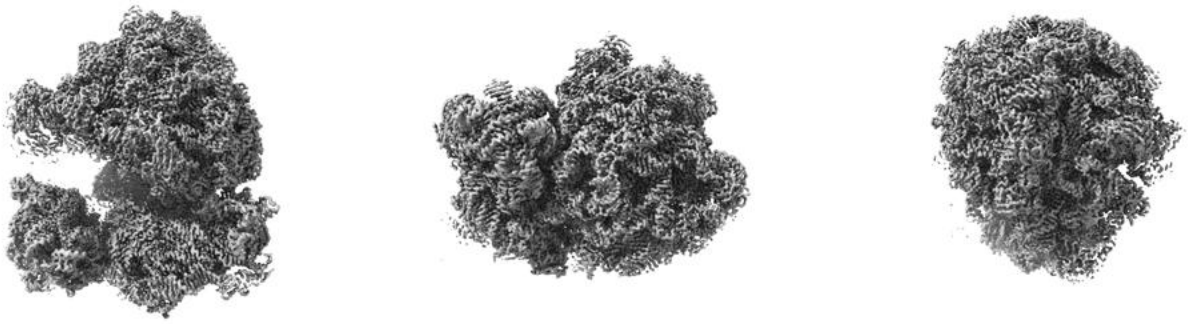


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

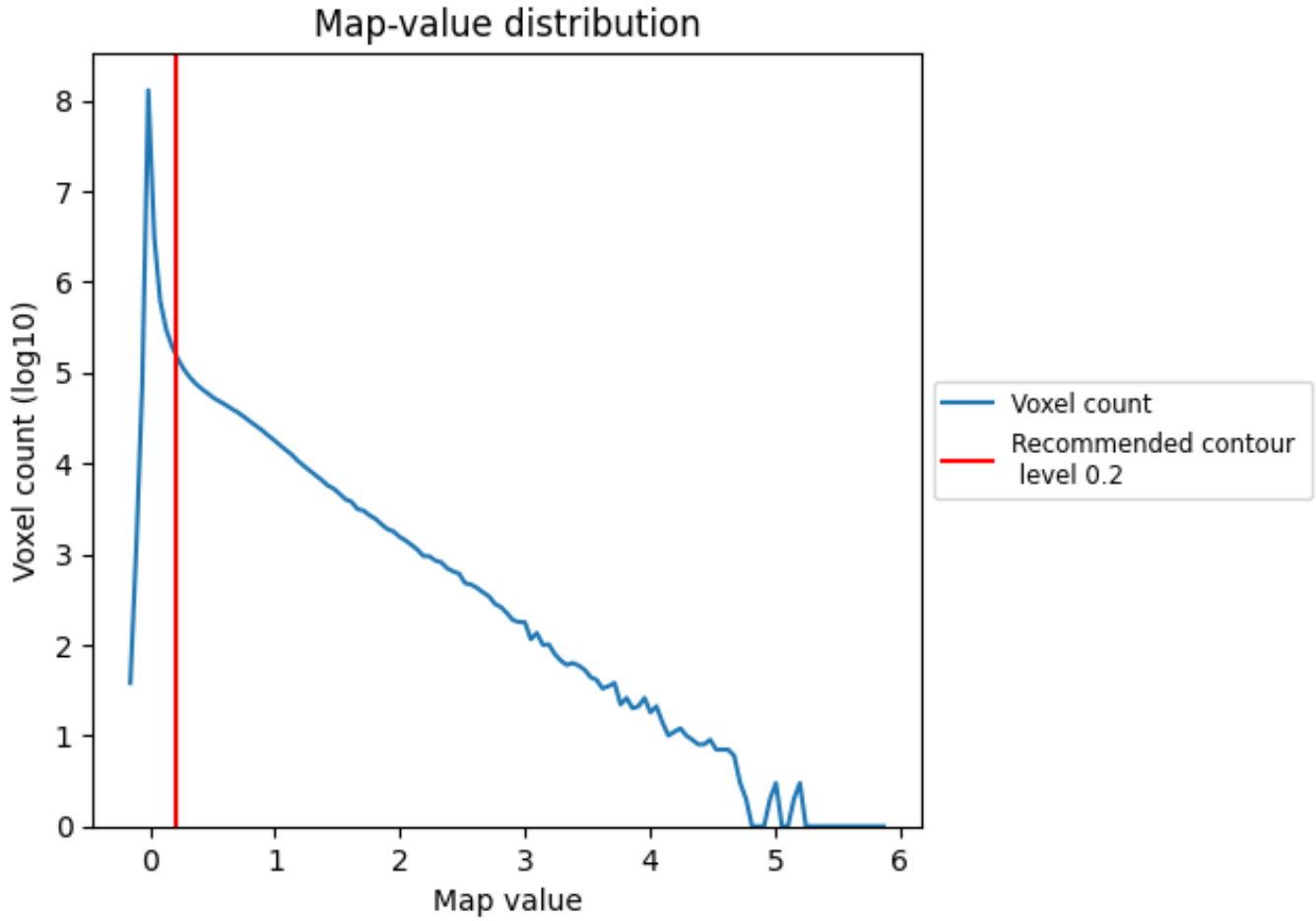
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

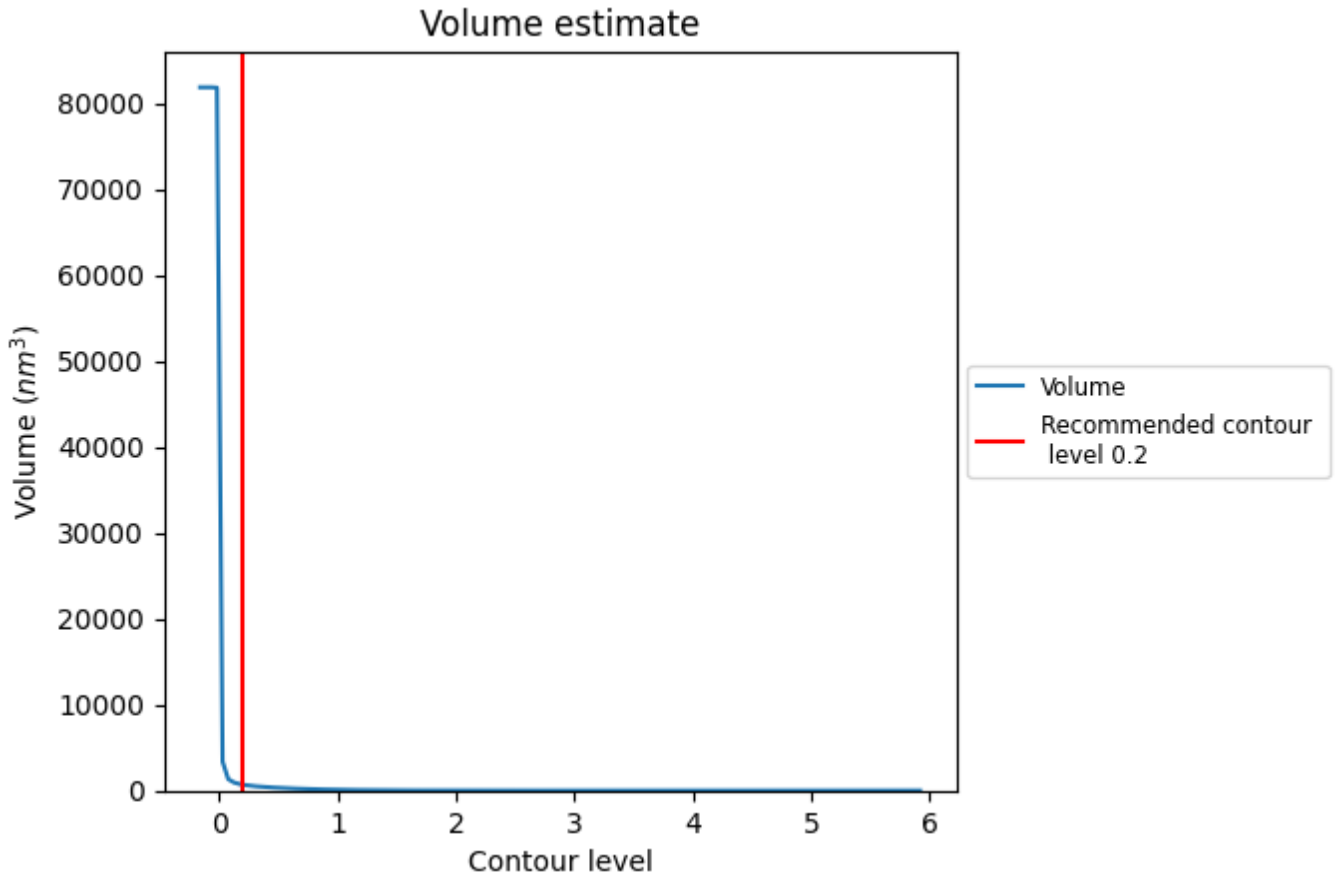
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

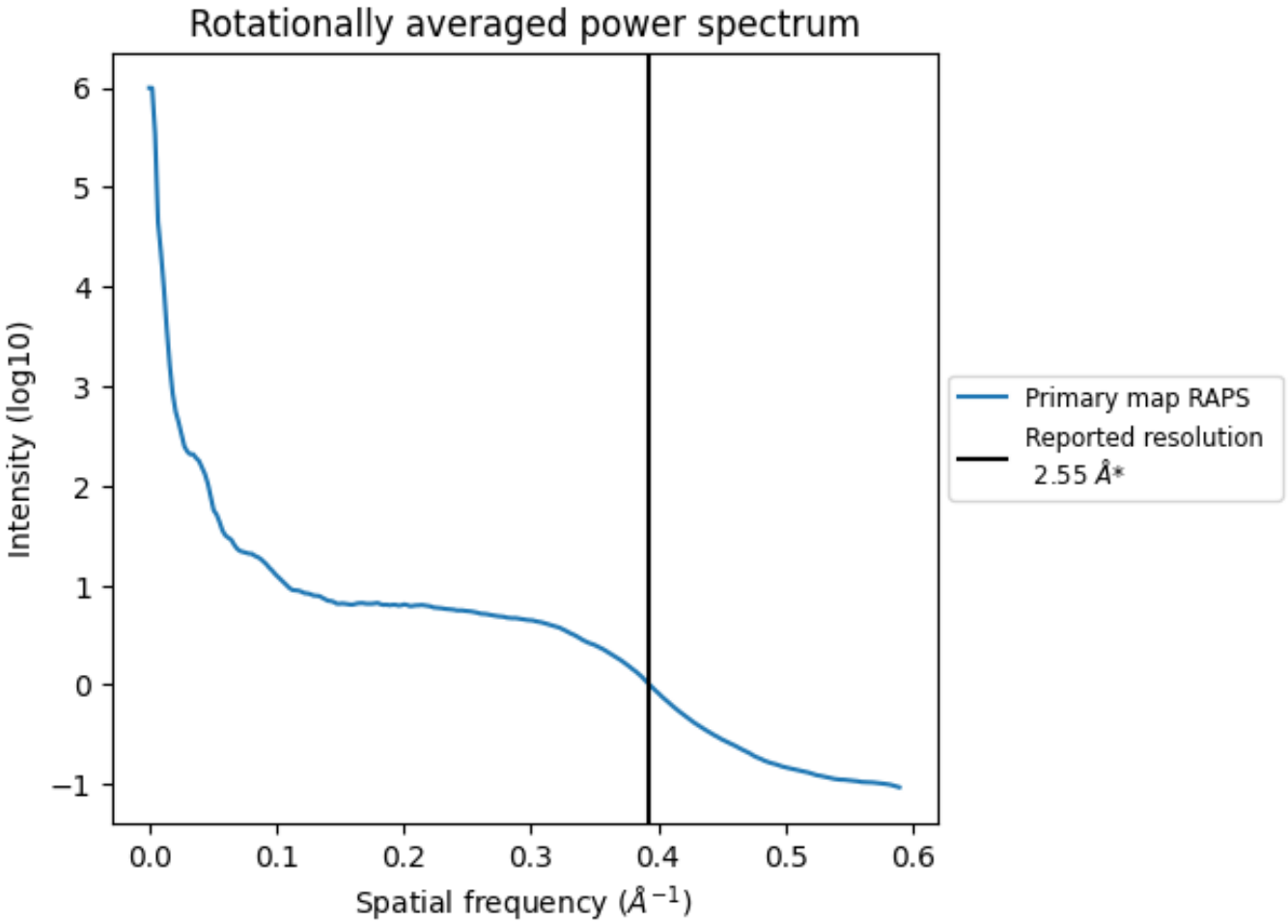
7.2 Volume estimate



The volume at the recommended contour level is 696 nm^3; this corresponds to an approximate mass of 629 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.392 Å^{-1}

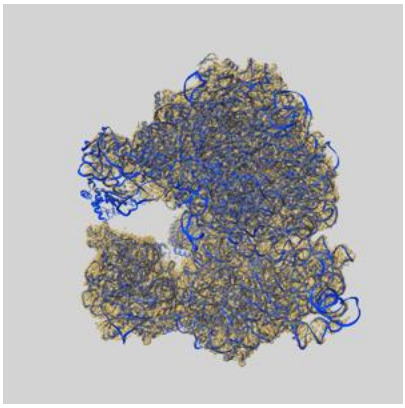
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

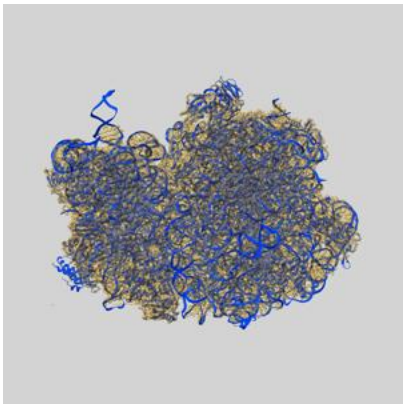
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23668 and PDB model 7M4W. Per-residue inclusion information can be found in section 3 on page 15.

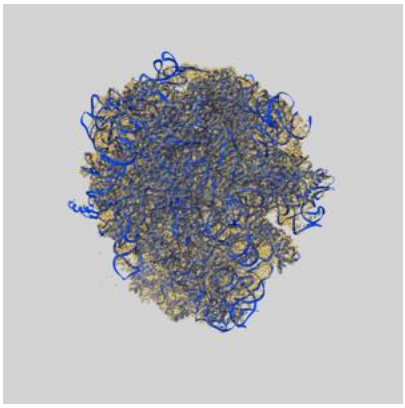
9.1 Map-model overlay



X



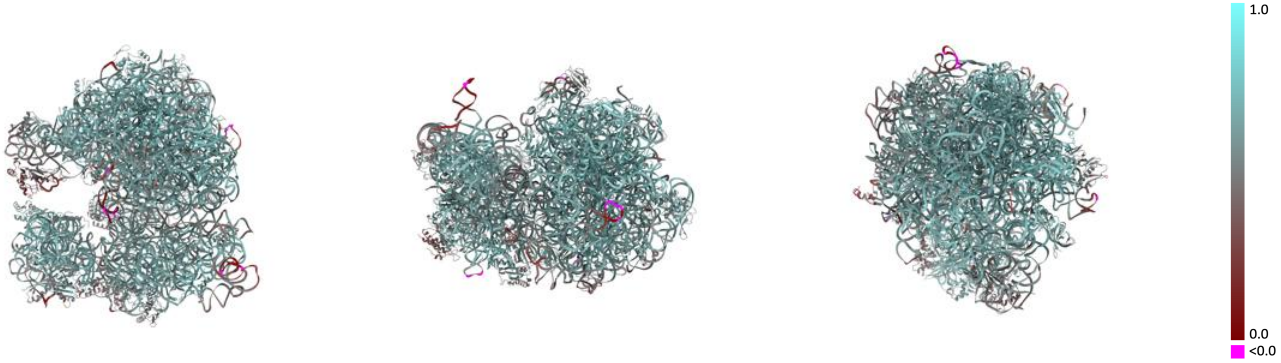
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

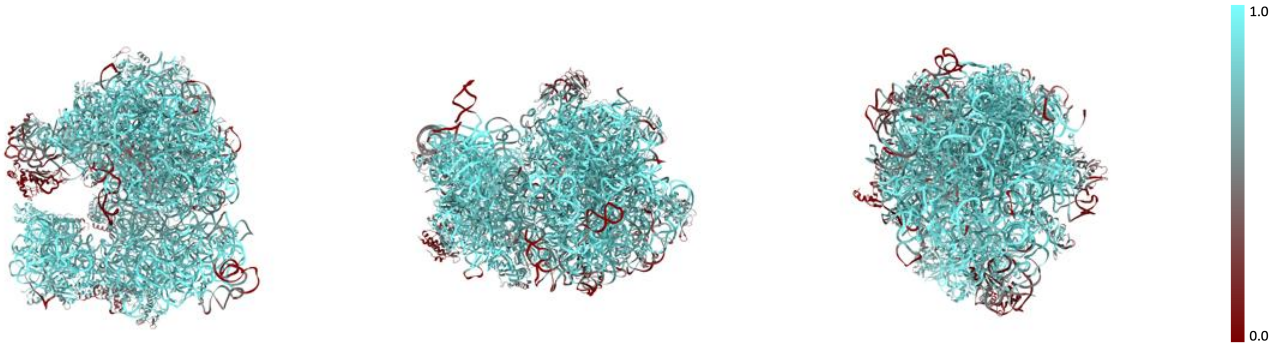
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

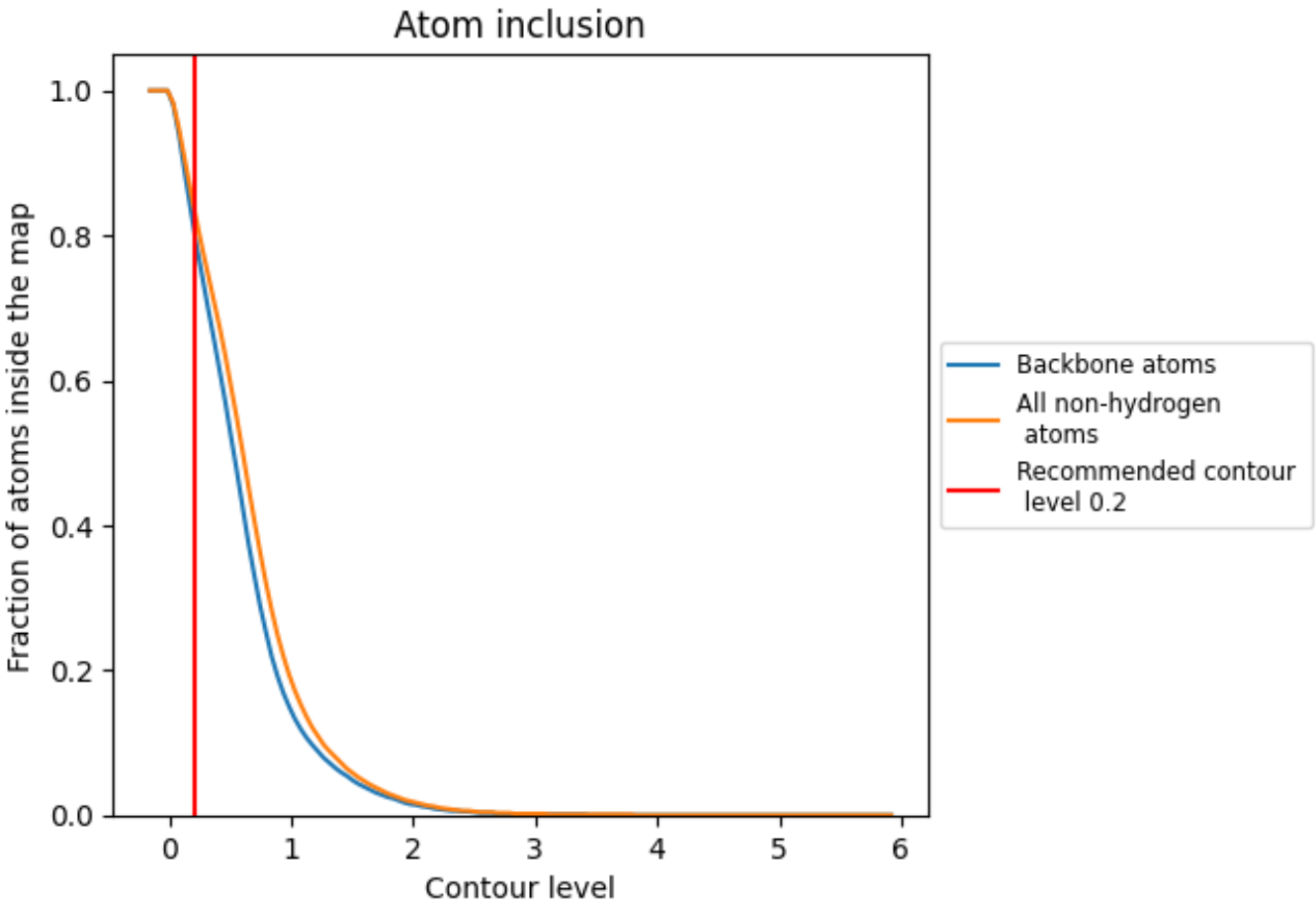
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8390	0.6120
0	0.7910	0.6360
1	0.9530	0.7180
2	0.9800	0.7220
3	0.8530	0.6230
A	0.8640	0.6240
B	0.5830	0.5320
C	0.9160	0.6660
D	0.9110	0.6870
E	0.7970	0.6550
F	0.0580	0.3350
G	0.4850	0.5100
H	0.1630	0.4040
I	0.9180	0.7000
J	0.8930	0.6550
K	0.8990	0.6880
L	0.8360	0.6310
M	0.9550	0.7030
N	0.5400	0.5400
O	0.8370	0.6400
P	0.9410	0.7070
Q	0.8380	0.6690
R	0.9110	0.6980
S	0.7340	0.6250
T	0.5490	0.5460
U	0.7110	0.5970
V	0.9120	0.7000
W	0.8500	0.6680
X	0.5100	0.5290
Y	0.8670	0.6710
Z	0.8090	0.6510
a	0.9090	0.6070
b	0.2300	0.3680
c	0.8960	0.6110
d	0.6970	0.5310



Continued on next page...

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Chain	Atom inclusion	Q-score
e	0.8820	0.6250
f	0.6980	0.5220
g	0.6750	0.4630
h	0.9300	0.6690
i	0.9180	0.6300
j	0.8700	0.6240
k	0.6960	0.5080
l	0.8580	0.6090
m	0.9230	0.6230
n	0.9320	0.6660
o	0.9280	0.6510
p	0.9020	0.6660
q	0.7610	0.5510
r	0.8890	0.6160
s	0.9570	0.6770
t	0.9060	0.6250
u	0.4080	0.4460